



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2017 – 06:38 PM EST

PDB ID : 5ISF
Title : Crystal structure of mouse CARM1 in complex with inhibitor SA0705
Authors : Cura, V.; Marechal, N.; Mailliot, J.; Troffer-Charlier, N.; Hassenboehler, P.; Wurtz, J.M.; Bonnefond, L.; Cavarelli, J.
Deposited on : 2016-03-15
Resolution : 2.22 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

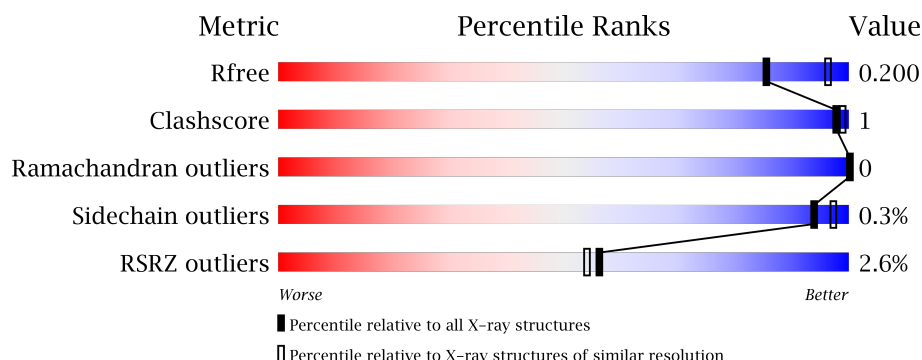
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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}	100719	4744 (2.24-2.20)
Clashscore	112137	5509 (2.24-2.20)
Ramachandran outliers	110173	5427 (2.24-2.20)
Sidechain outliers	110143	5428 (2.24-2.20)
RSRZ outliers	101464	4776 (2.24-2.20)

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 $\leq 5\%$. 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	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 1% 94% 5% </div> </div>
1	B	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 1%, green 95%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 2% 92% 5% </div> </div>
1	C	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 4%, yellow 1%, green 91%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 4% 93% 5% </div> </div>
1	D	361	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 3%, yellow 1%, green 93%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; font-size: 8px;"> 3% 93% 5% </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	503	-	-	-	X
4	PEG	A	503	-	-	-	X
5	PG4	A	505	-	-	-	X
5	PG4	B	506	-	-	-	X
7	DXE	B	504	-	-	-	X
7	DXE	C	504	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22818 atoms, of which 11128 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.

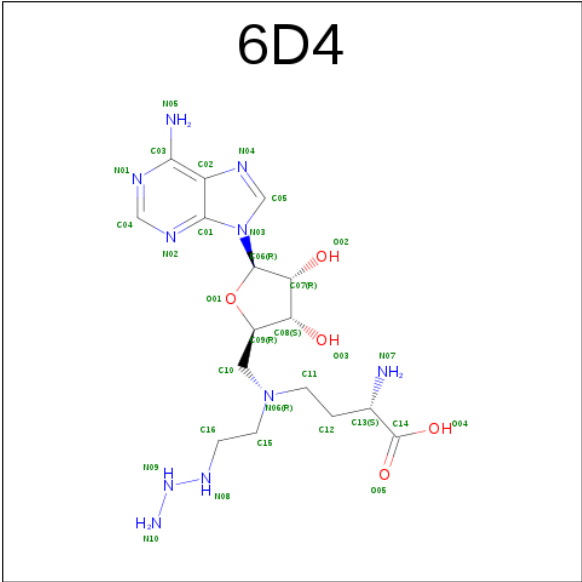
- Molecule 1 is a protein called Histone-arginine methyltransferase CARM1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	H	N	O	S	0	4	0
			5520	1796	2734	461	513	16			
1	B	343	Total	C	H	N	O	S	0	1	0
			5467	1781	2708	455	508	15			
1	C	343	Total	C	H	N	O	S	0	1	0
			5467	1781	2708	455	508	15			
1	D	343	Total	C	H	N	O	S	0	3	0
			5479	1784	2712	458	511	14			

There are 12 discrepancies between the modelled and reference sequences:

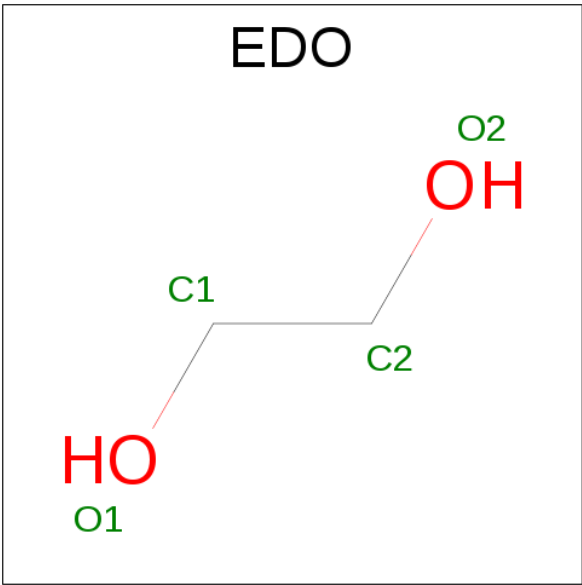
Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	expression tag	UNP Q9WVG6
A	128	HIS	-	expression tag	UNP Q9WVG6
A	129	MET	-	expression tag	UNP Q9WVG6
B	127	GLY	-	expression tag	UNP Q9WVG6
B	128	HIS	-	expression tag	UNP Q9WVG6
B	129	MET	-	expression tag	UNP Q9WVG6
C	127	GLY	-	expression tag	UNP Q9WVG6
C	128	HIS	-	expression tag	UNP Q9WVG6
C	129	MET	-	expression tag	UNP Q9WVG6
D	127	GLY	-	expression tag	UNP Q9WVG6
D	128	HIS	-	expression tag	UNP Q9WVG6
D	129	MET	-	expression tag	UNP Q9WVG6

- Molecule 2 is 5'-{[(3S)-3-amino-3-carboxypropyl][2-(triazan-1-yl)ethyl]amino}-5'-deoxyadenosine (three-letter code: 6D4) (formula: C₁₆H₂₈N₁₀O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			55	16	24	10	5		
2	B	1	Total	C	H	N	O	0	0
			55	16	24	10	5		
2	D	1	Total	C	H	N	O	0	0
			55	16	24	10	5		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



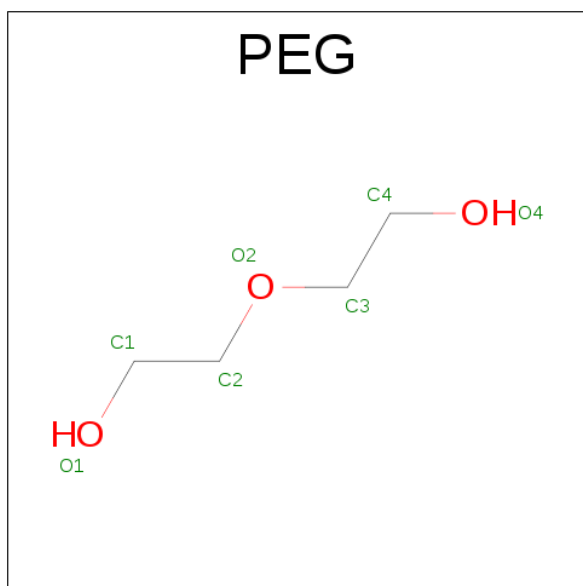
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		

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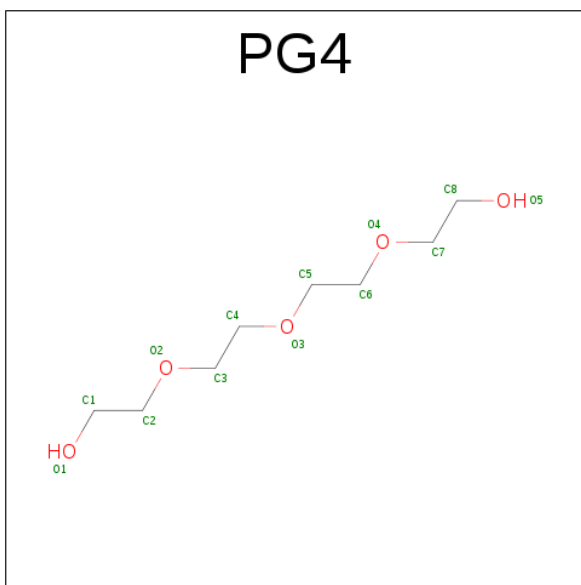
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



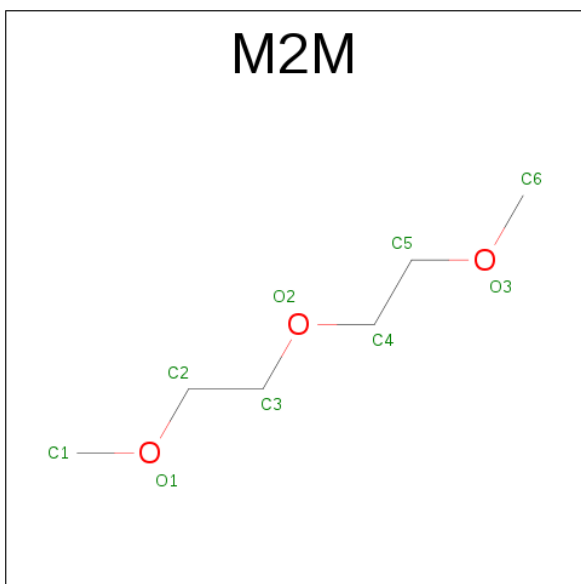
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



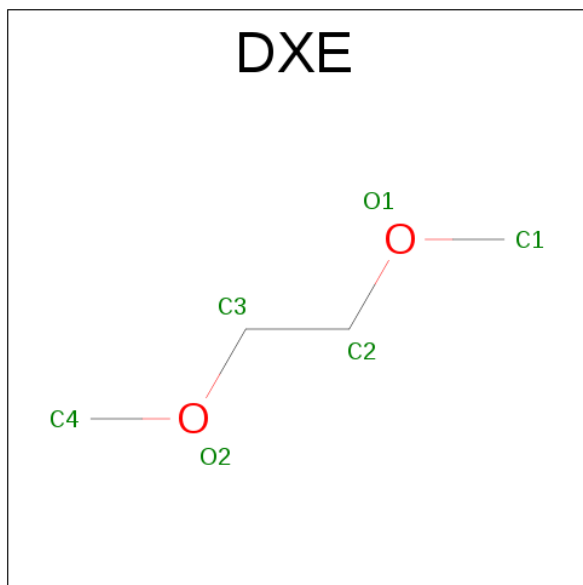
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			31	8	18	5		
5	A	1	Total	C	H	O	0	0
			31	8	18	5		
5	B	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is 1-METHOXY-2-(2-METHOXYETHOXY)ETHANE (three-letter code: M2M) (formula: C₆H₁₄O₃).



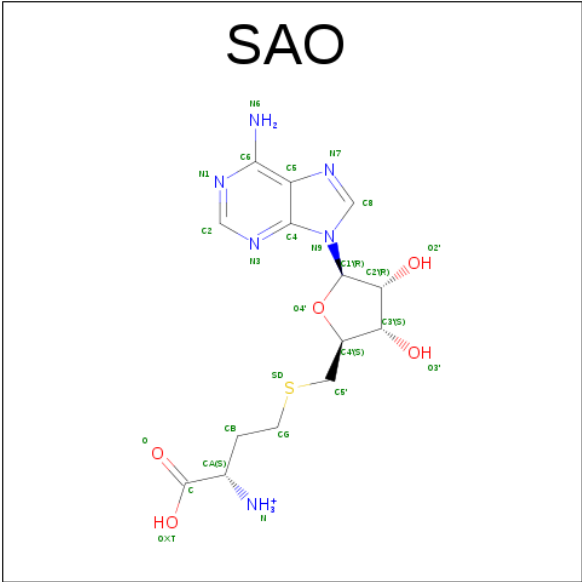
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			23	6	14	3		
6	C	1	Total	C	H	O	0	0
			23	6	14	3		

- Molecule 7 is 1,2-DIMETHOXYETHANE (three-letter code: DXE) (formula: C₄H₁₀O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			16	4	10	2		
7	B	1	Total	C	H	O	0	0
			16	4	10	2		
7	B	1	Total	C	H	O	0	0
			16	4	10	2		
7	C	1	Total	C	H	O	0	0
			16	4	10	2		

- Molecule 8 is 5'-S-[(3S)-3-azaniumyl-3-carboxypropyl]-5'-thioadenosine (three-letter code: SAO) (formula: C₁₄H₂₁N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	H	N	O	0	0
			46	14	20	6	5		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	128	Total	O	0	0
			128	128		
9	B	100	Total	O	0	0
			100	100		
9	C	91	Total	O	0	0
			91	91		
9	D	65	Total	O	0	0
			65	65		

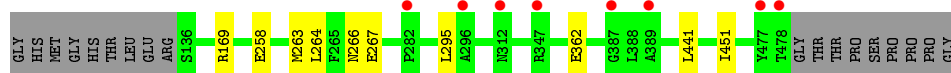
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

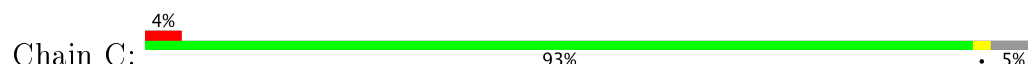
- Molecule 1: Histone-arginine methyltransferase CARM1



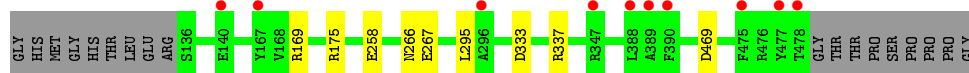
- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



- Molecule 1: Histone-arginine methyltransferase CARM1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.74Å 98.14Å 206.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.22 20.19 – 2.22	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.22) 97.2 (20.19-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.12 (at 2.21Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1980)	Depositor
R, R_{free}	0.166 , 0.201 0.162 , 0.200	Depositor DCC
R_{free} test set	3647 reflections (4.95%)	DCC
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22818	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.38 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.0437e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: SAO, 6D4, EDO, M2M, PG4, DXE, PEG

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	0.24	0/2856	0.39	0/3868
1	B	0.23	0/2829	0.38	0/3833
1	C	0.23	0/2829	0.37	0/3833
1	D	0.23	0/2845	0.38	0/3857
All	All	0.23	0/11359	0.38	0/15391

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2786	2734	2730	2	0
1	B	2759	2708	2707	5	0
1	C	2759	2708	2707	6	0
1	D	2767	2712	2699	6	0
2	A	31	24	0	0	0
2	B	31	24	0	0	0
2	D	31	24	0	1	0
3	A	4	6	6	0	0
3	B	8	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	12	12	0	0
3	D	8	12	12	0	0
4	A	7	10	10	0	0
5	A	26	36	36	0	0
5	B	13	18	18	0	0
6	A	9	14	14	0	0
6	C	9	14	14	0	0
7	A	6	10	10	0	0
7	B	12	20	20	0	0
7	C	6	10	10	0	0
8	C	26	20	0	0	0
9	A	128	0	0	1	0
9	B	100	0	0	1	0
9	C	91	0	0	4	0
9	D	65	0	0	2	0
All	All	11690	11128	11017	19	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 1.

All (19) 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:169:ARG:NH1	1:D:258:GLU:OE2	2.09	0.84
1:B:362:GLU:OE2	9:B:601:HOH:O	2.02	0.76
1:C:159:GLN:OE1	9:C:601:HOH:O	2.08	0.71
1:D:175:ARG:NH2	9:D:602:HOH:O	2.22	0.71
1:B:169:ARG:NH1	1:B:258:GLU:OE2	2.27	0.68
1:A:469:ASP:OD1	9:A:601:HOH:O	2.12	0.67
1:D:469:ASP:OD1	9:D:601:HOH:O	2.17	0.58
1:C:302:GLN:NE2	9:C:604:HOH:O	2.37	0.58
1:D:169:ARG:NH1	2:D:501:6D4:O05	2.36	0.56
1:D:333:ASP:O	1:D:337:ARG:HG3	2.13	0.48
1:C:469:ASP:OD1	9:C:602:HOH:O	2.20	0.48
1:B:266:ASN:O	1:B:267:GLU:HB2	2.14	0.47
1:A:266:ASN:O	1:A:267:GLU:HB2	2.14	0.47
1:D:266:ASN:O	1:D:267:GLU:HB2	2.15	0.47
1:C:136:SER:N	9:C:608:HOH:O	2.49	0.44
1:C:266:ASN:O	1:C:267:GLU:HB2	2.17	0.44
1:B:441:LEU:HD23	1:B:451:ILE:HG12	2.00	0.42
1:C:263:MET:O	1:C:264:LEU:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:MET:O	1:B:264:LEU:HB3	2.20	0.41

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	345/361 (96%)	334 (97%)	11 (3%)	0	100	100
1	B	342/361 (95%)	333 (97%)	9 (3%)	0	100	100
1	C	342/361 (95%)	331 (97%)	11 (3%)	0	100	100
1	D	344/361 (95%)	335 (97%)	9 (3%)	0	100	100
All	All	1373/1444 (95%)	1333 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/313 (97%)	302 (100%)	1 (0%)	94	97
1	B	300/313 (96%)	299 (100%)	1 (0%)	94	97
1	C	300/313 (96%)	299 (100%)	1 (0%)	94	97
1	D	302/313 (96%)	301 (100%)	1 (0%)	94	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1205/1252 (96%)	1201 (100%)	4 (0%)	94 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
1	B	295	LEU
1	C	258	GLU
1	D	295	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

21 ligands 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	$\# Z > 2$
2	6D4	A	501	-	24,33,33	4.70	11 (45%)	21,46,46	1.95	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	502	-	3,3,3	0.47	0	2,2,2	0.49	0
4	PEG	A	503	-	6,6,6	0.49	0	5,5,5	0.80	0
5	PG4	A	504	-	12,12,12	0.52	0	11,11,11	0.50	0
5	PG4	A	505	-	12,12,12	0.54	0	11,11,11	0.35	0
6	M2M	A	506	-	8,8,8	0.59	0	7,7,7	0.26	0
7	DXE	A	507	-	5,5,5	0.38	0	4,4,4	0.19	0
2	6D4	B	501	-	24,33,33	4.67	11 (45%)	21,46,46	1.89	3 (14%)
3	EDO	B	502	-	3,3,3	0.47	0	2,2,2	0.48	0
3	EDO	B	503	-	3,3,3	0.47	0	2,2,2	0.51	0
7	DXE	B	504	-	5,5,5	0.42	0	4,4,4	0.21	0
7	DXE	B	505	-	5,5,5	0.43	0	4,4,4	0.18	0
5	PG4	B	506	-	12,12,12	0.53	0	11,11,11	0.50	0
8	SAO	C	501	-	22,28,28	0.53	0	21,40,40	1.13	1 (4%)
3	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.52	0
3	EDO	C	503	-	3,3,3	0.48	0	2,2,2	0.50	0
7	DXE	C	504	-	5,5,5	0.41	0	4,4,4	0.20	0
6	M2M	C	505	-	8,8,8	0.60	0	7,7,7	0.24	0
2	6D4	D	501	-	24,33,33	4.69	11 (45%)	21,46,46	1.92	4 (19%)
3	EDO	D	502	-	3,3,3	0.47	0	2,2,2	0.49	0
3	EDO	D	503	-	3,3,3	0.47	0	2,2,2	0.51	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
2	6D4	A	501	-	-	0/12/38/38	0/3/3/3
3	EDO	A	502	-	-	0/1/1/1	0/0/0/0
4	PEG	A	503	-	-	0/4/4/4	0/0/0/0
5	PG4	A	504	-	-	0/10/10/10	0/0/0/0
5	PG4	A	505	-	-	0/10/10/10	0/0/0/0
6	M2M	A	506	-	-	0/6/6/6	0/0/0/0
7	DXE	A	507	-	-	0/3/3/3	0/0/0/0
2	6D4	B	501	-	-	0/12/38/38	0/3/3/3
3	EDO	B	502	-	-	0/1/1/1	0/0/0/0
3	EDO	B	503	-	-	0/1/1/1	0/0/0/0
7	DXE	B	504	-	-	0/3/3/3	0/0/0/0
7	DXE	B	505	-	-	0/3/3/3	0/0/0/0
5	PG4	B	506	-	-	0/10/10/10	0/0/0/0
8	SAO	C	501	-	-	0/7/31/31	0/3/3/3
3	EDO	C	502	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	503	-	-	0/1/1/1	0/0/0/0
7	DXE	C	504	-	-	0/3/3/3	0/0/0/0
6	M2M	C	505	-	-	0/6/6/6	0/0/0/0
2	6D4	D	501	-	-	0/12/38/38	0/3/3/3
3	EDO	D	502	-	-	0/1/1/1	0/0/0/0
3	EDO	D	503	-	-	0/1/1/1	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6D4	C16-N08	-18.73	1.26	1.45
2	D	501	6D4	C16-N08	-18.65	1.26	1.45
2	B	501	6D4	C16-N08	-18.61	1.26	1.45
2	A	501	6D4	N10-N09	-4.59	1.22	1.41
2	D	501	6D4	N10-N09	-4.57	1.22	1.41
2	B	501	6D4	N10-N09	-4.50	1.23	1.41
2	D	501	6D4	C07-C06	-3.48	1.48	1.53
2	A	501	6D4	C07-C06	-3.46	1.48	1.53
2	B	501	6D4	C07-C06	-3.45	1.48	1.53
2	B	501	6D4	C08-C07	-2.64	1.46	1.53
2	B	501	6D4	C08-C09	-2.40	1.46	1.53
2	A	501	6D4	C08-C07	-2.39	1.47	1.53
2	D	501	6D4	C08-C07	-2.30	1.47	1.53
2	D	501	6D4	C08-C09	-2.28	1.47	1.53
2	A	501	6D4	C08-C09	-2.25	1.47	1.53
2	B	501	6D4	C12-C11	2.26	1.57	1.52
2	D	501	6D4	C12-C11	2.52	1.58	1.52
2	A	501	6D4	C12-C11	2.57	1.58	1.52
2	D	501	6D4	C04-N02	2.78	1.36	1.32
2	A	501	6D4	C04-N02	2.78	1.36	1.32
2	B	501	6D4	C04-N02	2.83	1.36	1.32
2	A	501	6D4	C03-N05	3.28	1.47	1.34
2	B	501	6D4	C03-N05	3.29	1.47	1.34
2	D	501	6D4	C03-N05	3.32	1.47	1.34
2	A	501	6D4	O01-C09	3.33	1.52	1.45
2	D	501	6D4	O01-C09	3.40	1.52	1.45
2	B	501	6D4	O01-C09	3.53	1.53	1.45
2	A	501	6D4	C02-N04	3.92	1.52	1.39
2	D	501	6D4	C02-N04	3.92	1.52	1.39
2	B	501	6D4	C02-N04	3.97	1.52	1.39
2	B	501	6D4	O01-C06	7.87	1.52	1.41
2	D	501	6D4	O01-C06	8.12	1.52	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	6D4	O01-C06	8.16	1.52	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	6D4	C09-O01-C06	-6.17	103.20	109.77
2	B	501	6D4	C09-O01-C06	-6.02	103.36	109.77
2	D	501	6D4	C09-O01-C06	-5.47	103.95	109.77
2	D	501	6D4	C06-N03-C01	-4.66	118.58	126.64
2	A	501	6D4	C06-N03-C01	-4.36	119.11	126.64
8	C	501	SAO	CB-CG-SD	-4.21	105.45	113.57
2	B	501	6D4	C06-N03-C01	-4.06	119.63	126.64
2	A	501	6D4	C15-C16-N08	2.00	115.92	112.19
2	B	501	6D4	C07-C08-C09	2.30	107.09	102.62
2	D	501	6D4	C15-C16-N08	2.33	116.53	112.19
2	D	501	6D4	C07-C08-C09	2.77	108.02	102.62
2	A	501	6D4	C07-C08-C09	2.80	108.08	102.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	6D4	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 ⓘ

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, 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	343/361 (95%)	-0.31	5 (1%) 74 72	28, 40, 60, 90	0
1	B	343/361 (95%)	-0.21	8 (2%) 61 58	29, 44, 65, 100	0
1	C	343/361 (95%)	-0.13	13 (3%) 41 39	35, 50, 72, 105	0
1	D	343/361 (95%)	-0.09	10 (2%) 52 49	37, 50, 72, 114	0
All	All	1372/1444 (95%)	-0.19	36 (2%) 56 54	28, 47, 70, 114	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	477	TYR	6.4
1	D	478	THR	5.5
1	B	478	THR	5.2
1	A	478	THR	4.9
1	C	478	THR	3.8
1	B	477	TYR	3.5
1	C	477	TYR	3.3
1	C	256	ILE	3.0
1	C	282	PRO	3.0
1	D	347	ARG	3.0
1	D	388	LEU	2.9
1	C	140	GLU	2.9
1	D	389	ALA	2.9
1	D	475	PHE	2.8
1	A	477	TYR	2.8
1	D	390	PHE	2.6
1	C	191	ASP	2.6
1	B	312	ASN	2.6
1	D	167	TYR	2.6
1	D	140	GLU	2.5
1	B	282	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	197	GLY	2.4
1	A	197	GLY	2.3
1	A	347	ARG	2.3
1	C	231	ASN	2.3
1	C	136	SER	2.3
1	D	296	ALA	2.2
1	B	389	ALA	2.2
1	B	347	ARG	2.2
1	A	388	LEU	2.2
1	C	196	SER	2.2
1	B	387	GLY	2.2
1	B	296	ALA	2.1
1	C	221	GLN	2.1
1	C	199	LEU	2.0
1	C	347	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	PG4	A	505	13/13	0.78	0.38	9.79	65,78,80,80	0
4	PEG	A	503	7/7	0.86	0.22	3.98	60,72,79,79	0
7	DXE	C	504	6/6	0.88	0.29	3.60	62,74,78,78	0
7	DXE	B	504	6/6	0.86	0.20	3.15	63,75,84,84	0
5	PG4	B	506	13/13	0.76	0.22	2.42	62,74,82,84	0
3	EDO	B	503	4/4	0.88	0.31	2.32	58,70,74,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	M2M	A	506	9/9	0.82	0.23	1.97	60,72,79,82	0
6	M2M	C	505	9/9	0.82	0.21	1.70	63,76,85,87	0
5	PG4	A	504	13/13	0.92	0.16	1.56	56,69,85,85	0
7	DXE	B	505	6/6	0.85	0.18	1.35	61,73,80,80	0
2	6D4	D	501	31/31	0.92	0.14	0.69	39,56,87,99	0
3	EDO	A	502	4/4	0.88	0.18	0.64	60,72,74,77	0
2	6D4	A	501	31/31	0.92	0.14	0.27	31,45,77,92	0
3	EDO	D	503	4/4	0.78	0.16	0.26	63,76,77,79	0
3	EDO	C	503	4/4	0.85	0.15	0.03	60,72,74,74	0
2	6D4	B	501	31/31	0.96	0.12	-0.18	29,52,78,93	0
8	SAO	C	501	26/26	0.96	0.10	-0.71	42,52,67,68	0
3	EDO	D	502	4/4	0.90	0.15	-	58,70,71,73	0
3	EDO	B	502	4/4	0.86	0.14	-	48,58,61,67	0
7	DXE	A	507	6/6	0.88	0.28	-	39,47,53,53	0
3	EDO	C	502	4/4	0.90	0.14	-	60,72,74,77	0

6.5 Other polymers

There are no such residues in this entry.