WORLD WIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 11, 2024 – 08:34 PM EST

PDB ID	:	3DLH
Title	:	Crystal structure of the guide-strand-containing Argonaute protein silencing complex
Authors	:	Wang, Y.; Sheng, G.; Patel, D.J.
Deposited on	:	2008-06-27
Resolution	:	3.00 Å(reported)

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 3.00 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.
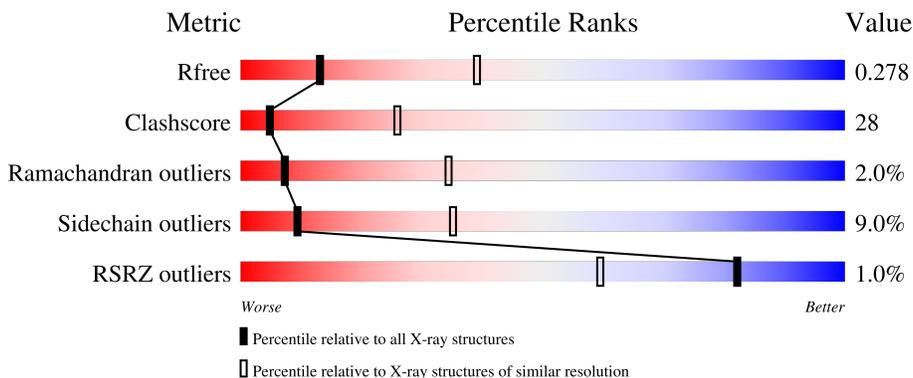
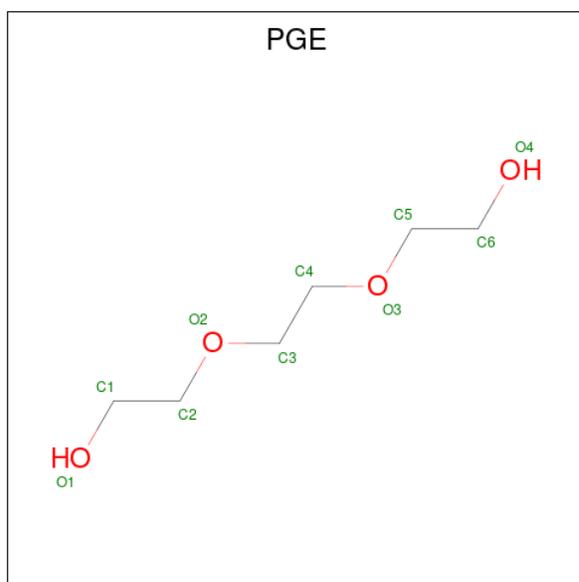| Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	685	% 53% 40% · ·
1	B	685	% 49% 42% 6% ·
2	X	21	10% 10% 62% 10% 19%
2	Y	21	5% 33% 29% 5% 33%

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
5	PO4	X	22	-	-	-	X
6	ACY	B	687	-	-	X	-

2   Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 10986 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 Argonaute.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	673	Total 5213	C 3337	N 973	O 896	S 7	63	0	0
1	B	666	Total 5079	C 3263	N 948	O 860	S 8	38	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DAP*DGP*DGP*DTP*DTP*DGP*DTP*DAP*DTP*DAP*DGP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	17	Total 329	C 155	N 60	O 98	P 16	0	0	1
2	Y	14	Total 259	C 120	N 48	O 78	P 13	0	0	1

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0
3	Y	1	Total 1	Mg 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

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PGE

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 6	O 4	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4
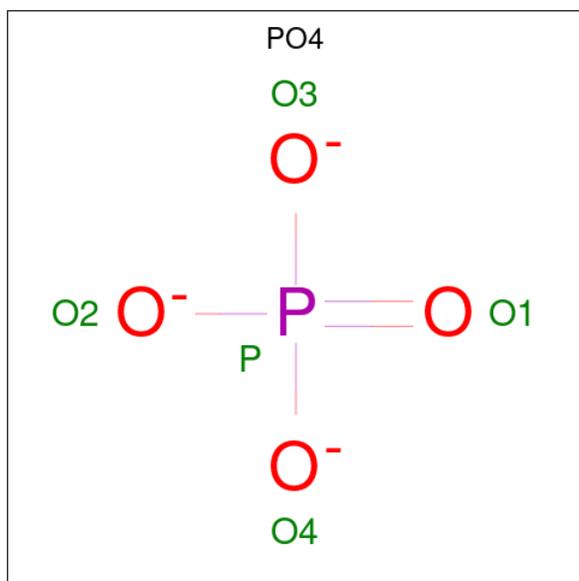
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0
5	X	1	Total 5	O 4	P 1	0	0

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).

ACY

OXT

OH

C

CH3

O

O
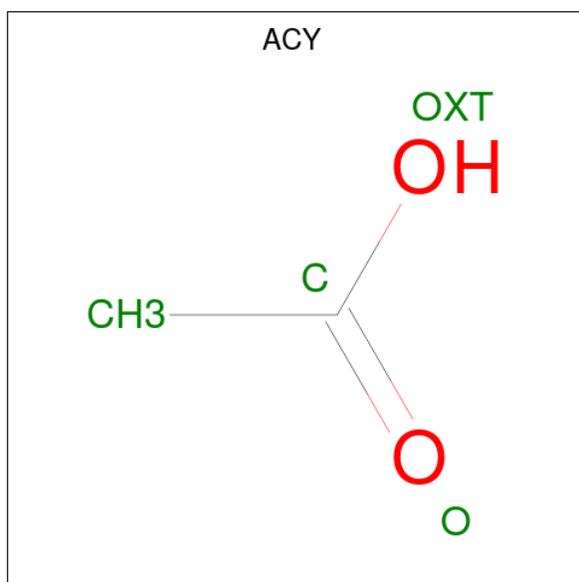
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total 4	C 2	O 2	0	0
6	B	1	Total 4	C 2	O 2	0	0

• Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total 39	O 39	0	0
7	B	35	Total 35	O 35	0	0
7	X	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Argonaute
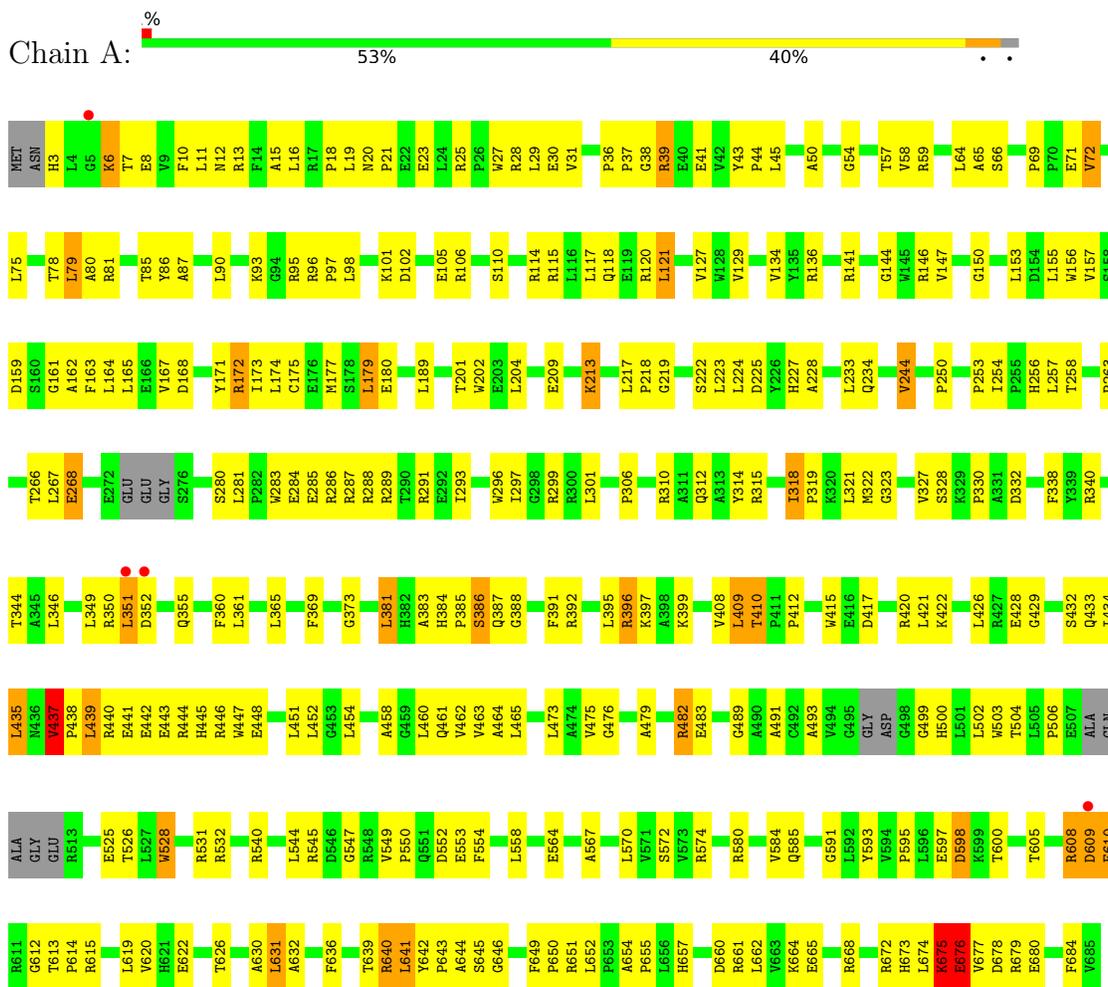
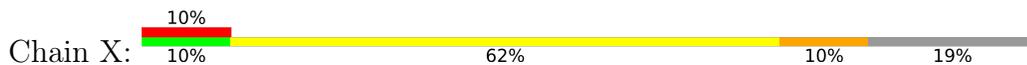

- Molecule 1: Argonaute
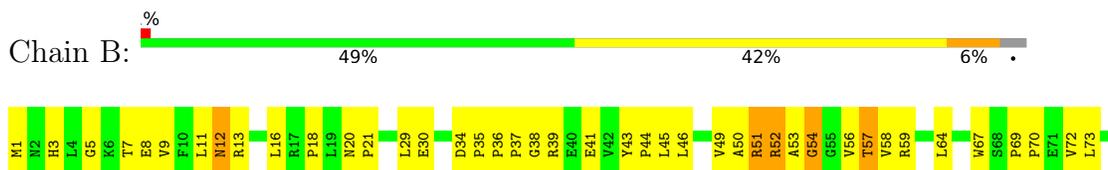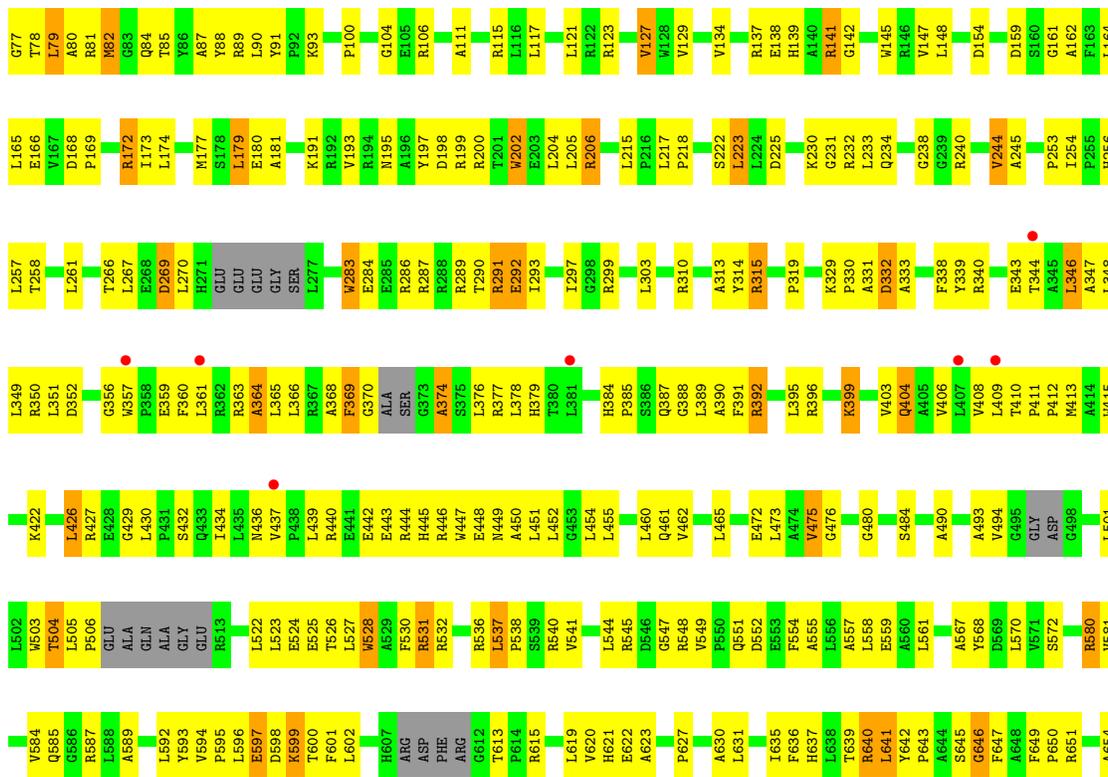
• Molecule 2: DNA (5'-D(DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DAP*DGP*D GP*DTP*DTP*DGP*DTP*DAP*DTP*DAP*DGP*DT)-3')

Chain X:

• Molecule 2: DNA (5'-D(DTP*DGP*DAP*DGP*DGP*DTP*DAP*DGP*DTP*DAP*DGP*D GP*DTP*DTP*DGP*DTP*DAP*DTP*DAP*DGP*DT)-3')

Chain Y:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.74Å 114.63Å 175.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 48.00 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-3.00) 90.9 (48.00-2.89)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.284 0.218 , 0.278	Depositor DCC
R_{free} test set	2323 reflections (6.97%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 57.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10986	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, PO4, PGE, ACY

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	0.47	2/5336 (0.0%)	0.77	14/7250 (0.2%)
1	B	0.44	0/5199	0.73	3/7071 (0.0%)
2	X	0.84	2/368 (0.5%)	1.04	0/565
2	Y	0.87	2/289 (0.7%)	0.88	0/444
All	All	0.49	6/11192 (0.1%)	0.77	17/15330 (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
1	A	0	3
2	X	0	1
2	Y	0	1
All	All	0	5

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	677	VAL	CB-CG1	-7.55	1.37	1.52
2	X	17	DA	O3'-P	-7.49	1.52	1.61
2	Y	101	DT	OP3-P	-7.30	1.52	1.61
2	Y	118	DT	O3'-P	-6.69	1.53	1.61
2	X	1	DT	OP3-P	-6.47	1.53	1.61

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	675	LYS	C-N-CA	-8.12	101.41	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	610	PHE	N-CA-C	8.07	132.78	111.00
1	A	677	VAL	N-CA-CB	7.46	127.92	111.50
1	A	677	VAL	CA-CB-CG2	7.45	122.08	110.90
1	B	384	HIS	N-CA-C	-6.72	92.86	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	608	ARG	Mainchain
1	A	609	ASP	Mainchain
1	A	676	GLU	Mainchain
2	X	7	DA	Sidechain
2	Y	104	DG	Sidechain

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	5213	0	5256	275	1
1	B	5079	0	5101	305	1
2	X	329	0	178	25	0
2	Y	259	0	137	14	0
3	A	2	0	0	0	0
3	Y	1	0	0	0	0
4	A	10	0	14	0	0
5	A	5	0	0	0	0
5	X	5	0	0	0	0
6	B	8	0	6	2	0
7	A	39	0	0	0	0
7	B	35	0	0	2	0
7	X	1	0	0	0	0
All	All	10986	0	10692	593	1

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 28.

The worst 5 of 593 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:B:525:GLU:HG2	1:B:679:ARG:HH12	1.03	1.13
1:A:280:SER:HA	2:X:7:DA:H5'	1.30	1.10
1:B:286:ARG:HD2	1:B:613:THR:HG21	1.12	1.09
1:A:327:VAL:HG23	1:A:332:ASP:HB2	1.28	1.09
1:B:138:GLU:CB	1:B:141:ARG:HH21	1.66	1.08

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:GLU:OE2	1:B:139:HIS:O[3_545]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	665/685 (97%)	601 (90%)	52 (8%)	12 (2%)	8	37
1	B	654/685 (96%)	569 (87%)	70 (11%)	15 (2%)	6	30
All	All	1319/1370 (96%)	1170 (89%)	122 (9%)	27 (2%)	7	34

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	355	GLN
1	B	39	ARG
1	B	374	ALA
1	B	597	GLU

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	512/549 (93%)	470 (92%)	42 (8%)	11	39
1	B	488/549 (89%)	440 (90%)	48 (10%)	8	30
All	All	1000/1098 (91%)	910 (91%)	90 (9%)	9	35

5 of 90 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	191	LYS
1	B	392	ARG
1	B	204	LEU
1	B	291	ARG
1	B	426	LEU

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	B	256	HIS
1	B	551	GLN
1	B	657	HIS
1	B	449	ASN
1	A	500	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	PGE	A	688	-	9,9,9	0.52	0	8,8,8	0.80	0
6	ACY	B	687	-	3,3,3	2.58	1 (33%)	3,3,3	0.72	0
6	ACY	B	686	-	3,3,3	2.58	1 (33%)	3,3,3	0.89	0
5	PO4	A	689	-	4,4,4	1.66	0	6,6,6	0.44	0
5	PO4	X	22	-	4,4,4	1.71	0	6,6,6	0.42	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	PGE	A	688	-	-	2/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	687	ACY	O-C	4.42	1.42	1.22
6	B	686	ACY	O-C	4.39	1.42	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

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Mol	Chain	Res	Type	Atoms
4	A	688	PGE	O3-C5-C6-O4
4	A	688	PGE	O2-C3-C4-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	687	ACY	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	672/685 (98%)	-0.26	4 (0%)	89	72	26, 52, 83, 95	18 (2%)
1	B	666/685 (97%)	-0.18	7 (1%)	80	56	25, 59, 89, 104	12 (1%)
2	X	17/21 (80%)	0.32	2 (11%)	4	1	32, 51, 150, 150	0
2	Y	14/21 (66%)	0.21	1 (7%)	16	5	55, 71, 129, 135	1 (7%)
All	All	1369/1412 (96%)	-0.21	14 (1%)	82	59	25, 56, 88, 150	31 (2%)

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	609	ASP	5.3
1	A	5	GLY	4.4
1	B	381	LEU	3.5
1	B	407	LEU	3.4
1	A	351	LEU	3.0

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 monosaccharides 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. 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	PO4	X	22	5/5	0.49	0.45	147,147,147,148	0
4	PGE	A	688	10/10	0.70	0.24	102,107,108,108	0
5	PO4	A	689	5/5	0.71	0.26	149,150,150,150	0
3	MG	A	687	1/1	0.87	0.15	57,57,57,57	0
6	ACY	B	687	4/4	0.90	0.30	60,61,61,62	0
6	ACY	B	686	4/4	0.93	0.24	44,45,45,46	0
3	MG	Y	2	1/1	0.96	0.11	26,26,26,26	0
3	MG	A	686	1/1	0.96	0.12	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.