wwPDB X-ray Structure Validation Summary Report (i)

Oct 6, 2024 – 12:41 pm BST

PDB ID	:	6Z3N
Title	:	Apo Structure of a Hydrolase from Pseudomonas aeruginosa PAO1
Authors	:	Jin, Y.; Rizkallah, P.; Bell, H.
Deposited on	:	2020-05-21
Resolution	:	1.58 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 (i) 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 (i)) were used in the production of this report:

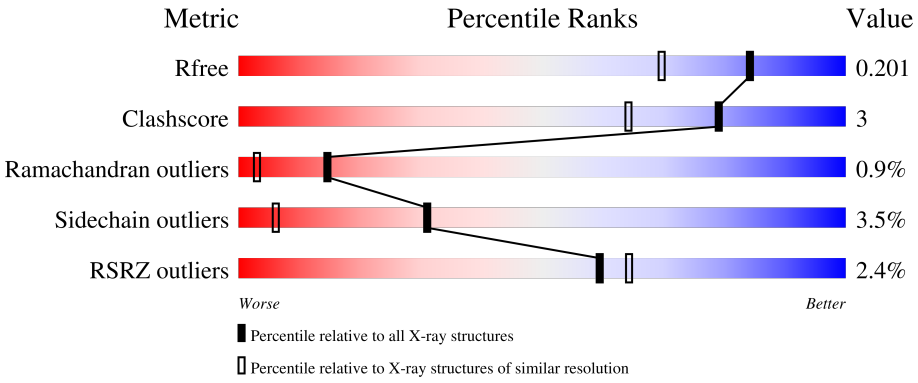
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 1.58 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}	164625	7165 (1.60-1.56)
Clashscore	180529	1026 (1.58-1.58)
Ramachandran outliers	177936	1005 (1.58-1.58)
Sidechain outliers	177891	1004 (1.58-1.58)
RSRZ outliers	164620	7163 (1.60-1.56)

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	AAA	205	78% 8% 14%
1	BBB	205	79% 7% 14%
1	CCC	205	80% 5% 14%
1	DDD	205	77% 7% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6228 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 Hydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	177	Total	C	N	O	S	Se	0	0	0
			1408	881	261	263	2	1			
1	BBB	177	Total	C	N	O	S	Se	0	1	0
			1417	886	263	265	2	1			
1	CCC	177	Total	C	N	O	S	Se	0	0	0
			1408	881	261	263	2	1			
1	DDD	177	Total	C	N	O	S	Se	0	0	0
			1408	881	261	263	2	1			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-20	MSE	-	initiating methionine	UNP Q9I686
AAA	-19	GLY	-	expression tag	UNP Q9I686
AAA	-18	SER	-	expression tag	UNP Q9I686
AAA	-17	SER	-	expression tag	UNP Q9I686
AAA	-16	HIS	-	expression tag	UNP Q9I686
AAA	-15	HIS	-	expression tag	UNP Q9I686
AAA	-14	HIS	-	expression tag	UNP Q9I686
AAA	-13	HIS	-	expression tag	UNP Q9I686
AAA	-12	HIS	-	expression tag	UNP Q9I686
AAA	-11	HIS	-	expression tag	UNP Q9I686
AAA	-10	SER	-	expression tag	UNP Q9I686
AAA	-9	SER	-	expression tag	UNP Q9I686
AAA	-8	GLY	-	expression tag	UNP Q9I686
AAA	-7	GLU	-	expression tag	UNP Q9I686
AAA	-6	ASN	-	expression tag	UNP Q9I686
AAA	-5	LEU	-	expression tag	UNP Q9I686
AAA	-4	TYR	-	expression tag	UNP Q9I686
AAA	-3	PHE	-	expression tag	UNP Q9I686
AAA	-2	GLN	-	expression tag	UNP Q9I686
AAA	-1	SER	-	expression tag	UNP Q9I686
AAA	0	HIS	-	expression tag	UNP Q9I686

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MSE	-	expression tag	UNP Q9I686
BBB	-20	MSE	-	initiating methionine	UNP Q9I686
BBB	-19	GLY	-	expression tag	UNP Q9I686
BBB	-18	SER	-	expression tag	UNP Q9I686
BBB	-17	SER	-	expression tag	UNP Q9I686
BBB	-16	HIS	-	expression tag	UNP Q9I686
BBB	-15	HIS	-	expression tag	UNP Q9I686
BBB	-14	HIS	-	expression tag	UNP Q9I686
BBB	-13	HIS	-	expression tag	UNP Q9I686
BBB	-12	HIS	-	expression tag	UNP Q9I686
BBB	-11	HIS	-	expression tag	UNP Q9I686
BBB	-10	SER	-	expression tag	UNP Q9I686
BBB	-9	SER	-	expression tag	UNP Q9I686
BBB	-8	GLY	-	expression tag	UNP Q9I686
BBB	-7	GLU	-	expression tag	UNP Q9I686
BBB	-6	ASN	-	expression tag	UNP Q9I686
BBB	-5	LEU	-	expression tag	UNP Q9I686
BBB	-4	TYR	-	expression tag	UNP Q9I686
BBB	-3	PHE	-	expression tag	UNP Q9I686
BBB	-2	GLN	-	expression tag	UNP Q9I686
BBB	-1	SER	-	expression tag	UNP Q9I686
BBB	0	HIS	-	expression tag	UNP Q9I686
BBB	1	MSE	-	expression tag	UNP Q9I686
CCC	-20	MSE	-	initiating methionine	UNP Q9I686
CCC	-19	GLY	-	expression tag	UNP Q9I686
CCC	-18	SER	-	expression tag	UNP Q9I686
CCC	-17	SER	-	expression tag	UNP Q9I686
CCC	-16	HIS	-	expression tag	UNP Q9I686
CCC	-15	HIS	-	expression tag	UNP Q9I686
CCC	-14	HIS	-	expression tag	UNP Q9I686
CCC	-13	HIS	-	expression tag	UNP Q9I686
CCC	-12	HIS	-	expression tag	UNP Q9I686
CCC	-11	HIS	-	expression tag	UNP Q9I686
CCC	-10	SER	-	expression tag	UNP Q9I686
CCC	-9	SER	-	expression tag	UNP Q9I686
CCC	-8	GLY	-	expression tag	UNP Q9I686
CCC	-7	GLU	-	expression tag	UNP Q9I686
CCC	-6	ASN	-	expression tag	UNP Q9I686
CCC	-5	LEU	-	expression tag	UNP Q9I686
CCC	-4	TYR	-	expression tag	UNP Q9I686
CCC	-3	PHE	-	expression tag	UNP Q9I686
CCC	-2	GLN	-	expression tag	UNP Q9I686

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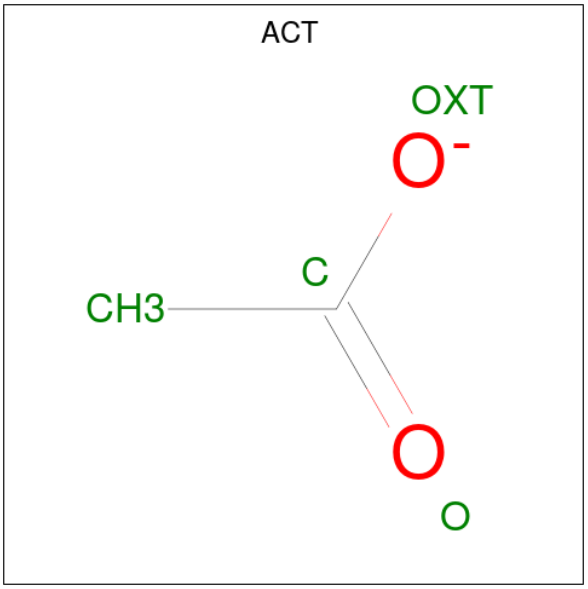
Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-1	SER	-	expression tag	UNP Q9I686
CCC	0	HIS	-	expression tag	UNP Q9I686
CCC	1	MSE	-	expression tag	UNP Q9I686
DDD	-20	MSE	-	initiating methionine	UNP Q9I686
DDD	-19	GLY	-	expression tag	UNP Q9I686
DDD	-18	SER	-	expression tag	UNP Q9I686
DDD	-17	SER	-	expression tag	UNP Q9I686
DDD	-16	HIS	-	expression tag	UNP Q9I686
DDD	-15	HIS	-	expression tag	UNP Q9I686
DDD	-14	HIS	-	expression tag	UNP Q9I686
DDD	-13	HIS	-	expression tag	UNP Q9I686
DDD	-12	HIS	-	expression tag	UNP Q9I686
DDD	-11	HIS	-	expression tag	UNP Q9I686
DDD	-10	SER	-	expression tag	UNP Q9I686
DDD	-9	SER	-	expression tag	UNP Q9I686
DDD	-8	GLY	-	expression tag	UNP Q9I686
DDD	-7	GLU	-	expression tag	UNP Q9I686
DDD	-6	ASN	-	expression tag	UNP Q9I686
DDD	-5	LEU	-	expression tag	UNP Q9I686
DDD	-4	TYR	-	expression tag	UNP Q9I686
DDD	-3	PHE	-	expression tag	UNP Q9I686
DDD	-2	GLN	-	expression tag	UNP Q9I686
DDD	-1	SER	-	expression tag	UNP Q9I686
DDD	0	HIS	-	expression tag	UNP Q9I686
DDD	1	MSE	-	expression tag	UNP Q9I686

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

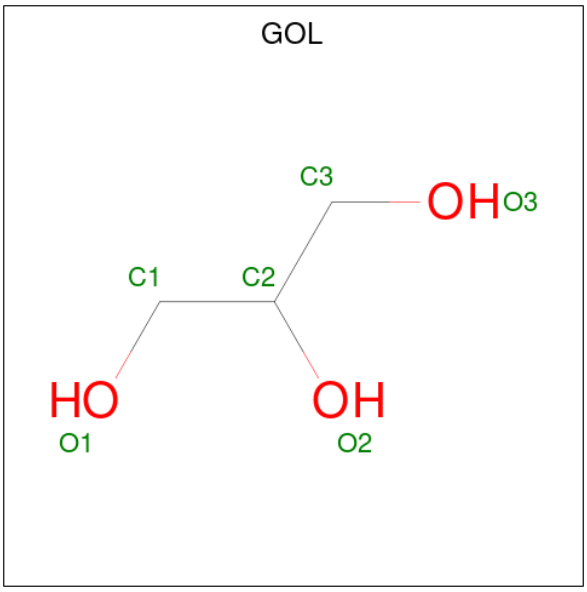


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total C O 4 2 2	0	0
2	CCC	1	Total C O 4 2 2	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Ni 1 1	0	0
3	BBB	1	Total Ni 1 1	0	0
3	CCC	1	Total Ni 1 1	0	0
3	DDD	1	Total Ni 1 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	CCC	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

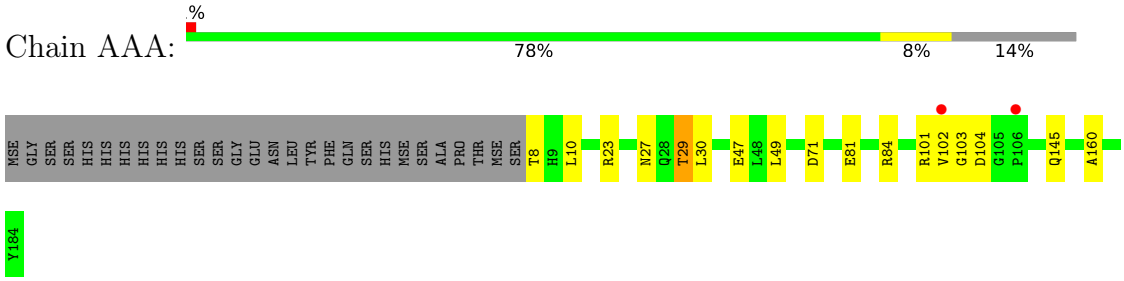
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	153	Total O 153 153	0	0
5	BBB	124	Total O 124 124	0	0
5	CCC	145	Total O 147 147	0	2
5	DDD	144	Total O 145 145	0	1

3 Residue-property plots (i)

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.

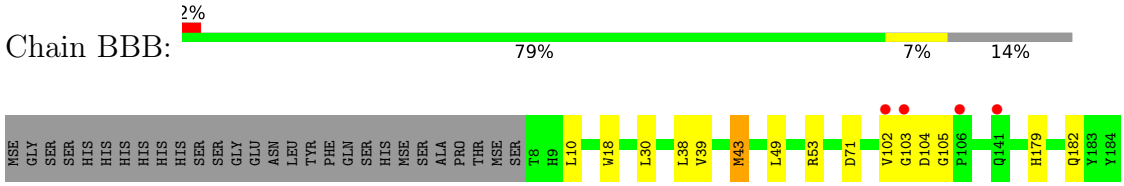
• Molecule 1: Hydrolase

Chain AAA:



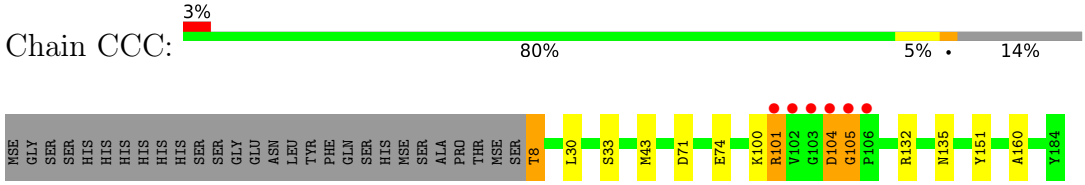
• Molecule 1: Hydrolase

Chain BBB:



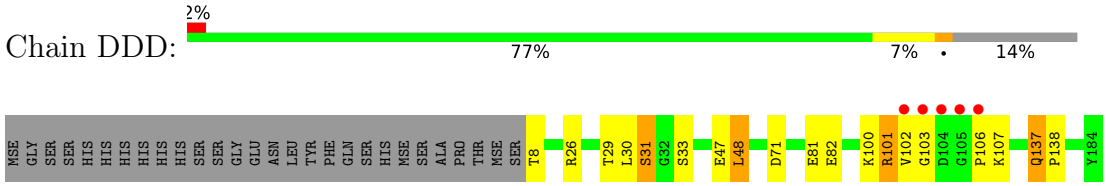
• Molecule 1: Hydrolase

Chain CCC:



• Molecule 1: Hydrolase

Chain DDD:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	85.31Å 85.90Å 122.64Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	59.90 – 1.58 59.90 – 1.58	Depositor EDS
% Data completeness (in resolution range)	81.2 (59.90-1.58) 81.2 (59.90-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.137 , 0.200 0.140 , 0.201	Depositor DCC
R_{free} test set	5991 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	6228	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 5.65% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ACT, NI

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	AAA	0.77	1/1438 (0.1%)	0.86	1/1951 (0.1%)
1	BBB	0.80	0/1447	0.88	2/1963 (0.1%)
1	CCC	0.80	0/1438	0.88	2/1951 (0.1%)
1	DDD	0.92	5/1438 (0.3%)	0.86	1/1951 (0.1%)
All	All	0.83	6/5761 (0.1%)	0.87	6/7816 (0.1%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	81	GLU	CD-OE1	11.63	1.38	1.25
1	DDD	81	GLU	CD-OE2	9.83	1.36	1.25
1	DDD	47	GLU	CD-OE1	8.92	1.35	1.25
1	DDD	47	GLU	CD-OE2	5.64	1.31	1.25
1	AAA	47	GLU	CD-OE1	5.08	1.31	1.25

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	43	MSE	CG-SE-CE	7.38	115.14	98.90
1	CCC	43	MSE	CG-SE-CE	5.93	111.95	98.90
1	AAA	27	ASN	CB-CA-C	5.80	122.00	110.40
1	DDD	48	LEU	CA-CB-CG	-5.68	102.24	115.30
1	CCC	132	ARG	NE-CZ-NH2	5.29	122.94	120.30

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	AAA	1408	0	1375	6	0
1	BBB	1417	0	1382	6	0
1	CCC	1408	0	1375	8	0
1	DDD	1408	0	1375	10	0
2	AAA	4	0	3	0	0
2	CCC	4	0	3	0	0
3	AAA	1	0	0	0	0
3	BBB	1	0	0	0	0
3	CCC	1	0	0	0	0
3	DDD	1	0	0	0	0
4	CCC	6	0	8	3	0
5	AAA	153	0	0	1	0
5	BBB	124	0	0	0	0
5	CCC	147	0	0	1	0
5	DDD	145	0	0	0	0
All	All	6228	0	5521	29	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 3.

The worst 5 of 29 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:DDD:101:ARG:HD3	1:DDD:106:PRO:C	2.21	0.61
1:DDD:102:VAL:HG13	1:DDD:103:GLY:N	2.15	0.61
1:BBB:39:VAL:HG12	1:BBB:43:MSE:HE2	1.86	0.56
1:BBB:103:GLY:C	1:BBB:105:GLY:H	2.11	0.54
1:CCC:104:ASP:O	1:CCC:105:GLY:O	2.27	0.53

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	AAA	175/205 (85%)	170 (97%)	4 (2%)	1 (1%)	22 7
1	BBB	176/205 (86%)	170 (97%)	4 (2%)	2 (1%)	12 1
1	CCC	175/205 (85%)	169 (97%)	4 (2%)	2 (1%)	12 1
1	DDD	175/205 (85%)	167 (95%)	7 (4%)	1 (1%)	22 7
All	All	701/820 (86%)	676 (96%)	19 (3%)	6 (1%)	14 3

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	103	GLY
1	CCC	105	GLY
1	BBB	104	ASP
1	BBB	102	VAL
1	CCC	104	ASP

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	AAA	144/165 (87%)	138 (96%)	6 (4%)	25 3
1	BBB	145/165 (88%)	143 (99%)	2 (1%)	62 39
1	CCC	144/165 (87%)	140 (97%)	4 (3%)	38 10
1	DDD	144/165 (87%)	136 (94%)	8 (6%)	17 2
All	All	577/660 (87%)	557 (96%)	20 (4%)	31 6

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	DDD	31	SER
1	DDD	101	ARG
1	DDD	137	GLN
1	DDD	107	LYS
1	BBB	30	LEU

Sometimes 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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 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	GOL	CCC	501	-	5,5,5	0.55	0	5,5,5	0.38	0
2	ACT	CCC	502	-	3,3,3	1.04	0	3,3,3	0.86	0
2	ACT	AAA	501	-	3,3,3	1.32	0	3,3,3	0.55	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	GOL	CCC	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	CCC	501	GOL	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

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	AAA	176/205 (85%)	-0.22	2 (1%)	77	82	20, 30, 73, 113	0
1	BBB	176/205 (85%)	-0.16	4 (2%)	61	66	15, 29, 67, 127	1 (0%)
1	CCC	176/205 (85%)	-0.09	6 (3%)	48	52	20, 30, 62, 144	3 (1%)
1	DDD	176/205 (85%)	-0.10	5 (2%)	55	59	20, 30, 69, 108	2 (1%)
All	All	704/820 (85%)	-0.14	17 (2%)	59	64	15, 30, 69, 144	6 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	106	PRO	6.7
1	DDD	103	GLY	6.2
1	CCC	105	GLY	5.6
1	DDD	104	ASP	5.4
1	CCC	102	VAL	4.8

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, 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	B-factors(Å^2)	Q<0.9
2	ACT	AAA	501	4/4	0.90	0.13	56,61,66,68	0
2	ACT	CCC	502	4/4	0.93	0.10	66,66,69,71	0
4	GOL	CCC	501	6/6	0.94	0.12	69,80,86,110	0
3	NI	DDD	201	1/1	0.95	0.12	61,61,61,61	1
3	NI	CCC	503	1/1	0.95	0.12	63,63,63,63	1
3	NI	BBB	201	1/1	0.98	0.07	56,56,56,56	1
3	NI	AAA	502	1/1	0.98	0.07	56,56,56,56	1

6.5 Other polymers (i)

There are no such residues in this entry.