



wwPDB X-ray Structure Validation Summary Report ⓘ

May 24, 2020 – 07:38 am BST

PDB ID : 3GZE
Title : Algal prolyl 4-hydroxylase complexed with zinc and (Ser-Pro)₅ peptide substrate
Authors : Koski, M.K.; Wierenga, R.K.
Deposited on : 2009-04-07
Resolution : 1.98 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 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	:	2.11
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)	:	2.11

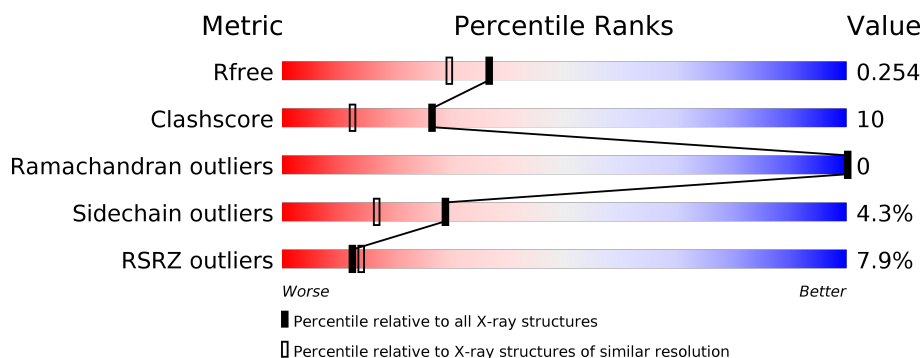
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 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	225	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>5%</div> </div> </div>
1	B	225	<div> <div>8%</div> <div> <div></div> <div>65%</div> <div>16%</div> <div>•</div> <div>17%</div> </div> </div>
1	C	225	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>•</div> <div>5%</div> </div> </div>
1	D	225	<div> <div>11%</div> <div> <div></div> <div>58%</div> <div>20%</div> <div>•</div> <div>19%</div> </div> </div>
2	X	10	<div> <div></div> <div> <div>40%</div> <div>20%</div> <div>40%</div> </div> </div>
2	Y	10	<div> <div></div> <div> <div>50%</div> <div>20%</div> <div>10%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6949 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 Predicted protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	5	0
			1699	1075	290	326	8			
1	B	186	Total	C	N	O	S	0	4	0
			1496	959	251	278	8			
1	C	213	Total	C	N	O	S	0	4	0
			1702	1075	293	326	8			
1	D	182	Total	C	N	O	S	0	2	0
			1459	933	248	270	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	EXPRESSION TAG	UNP A8J7D3
A	252	ARG	-	EXPRESSION TAG	UNP A8J7D3
A	253	HIS	-	EXPRESSION TAG	UNP A8J7D3
B	29	MET	-	EXPRESSION TAG	UNP A8J7D3
B	252	ARG	-	EXPRESSION TAG	UNP A8J7D3
B	253	HIS	-	EXPRESSION TAG	UNP A8J7D3
C	29	MET	-	EXPRESSION TAG	UNP A8J7D3
C	252	ARG	-	EXPRESSION TAG	UNP A8J7D3
C	253	HIS	-	EXPRESSION TAG	UNP A8J7D3
D	29	MET	-	EXPRESSION TAG	UNP A8J7D3
D	252	ARG	-	EXPRESSION TAG	UNP A8J7D3
D	253	HIS	-	EXPRESSION TAG	UNP A8J7D3

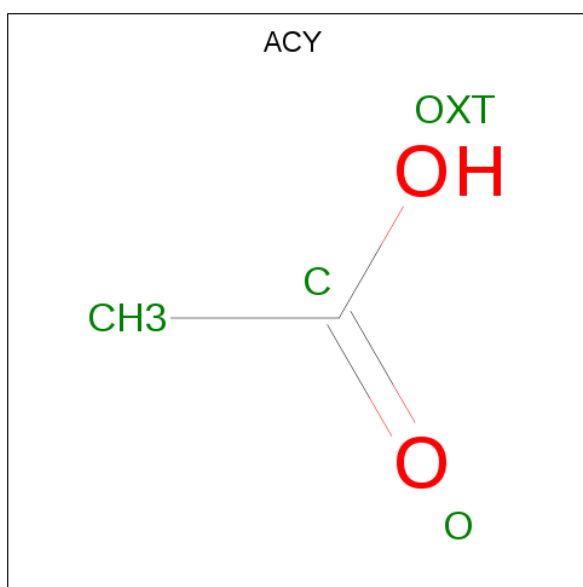
- Molecule 2 is a protein called Peptide substrate (Ser-Pro)5.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	0	0	0
			39	24	6	9			
2	Y	8	Total	C	N	O	0	0	0
			52	32	8	12			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Zn	0	0
			3	3		
3	A	5	Total	Zn	0	0
			5	5		
3	D	2	Total	Zn	0	0
			2	2		
3	C	4	Total	Zn	0	0
			4	4		

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

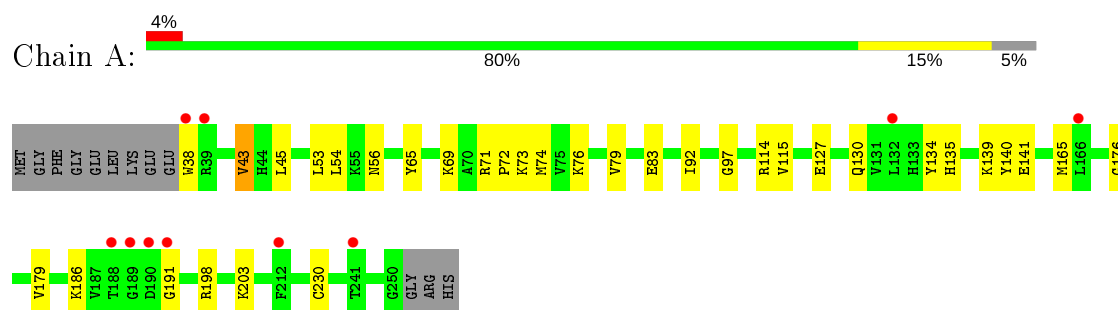
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	152	Total 152	O 152	0	0
5	B	108	Total 108	O 108	0	0
5	C	127	Total 127	O 127	0	0
5	D	74	Total 74	O 74	0	0
5	X	3	Total 3	O 3	0	0
5	Y	2	Total 2	O 2	0	0
5	Y	2	Total 2	O 2	0	0

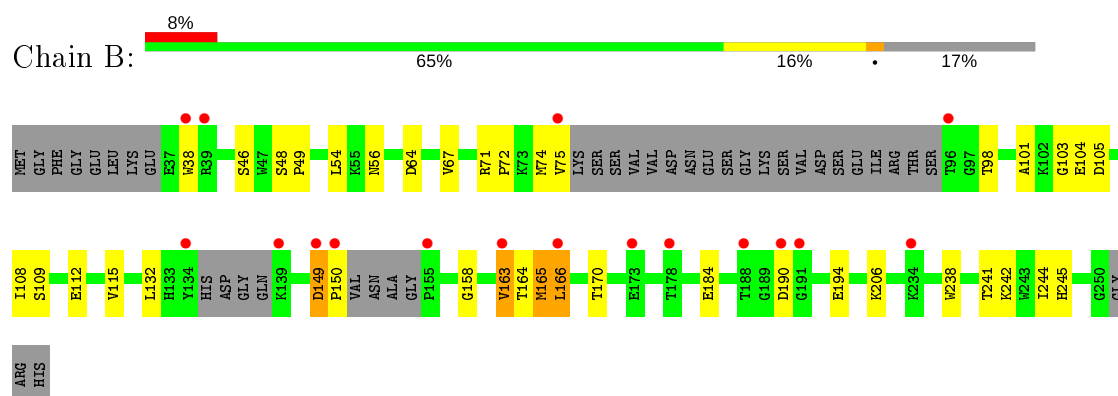
3 Residue-property plots [i](#)

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.

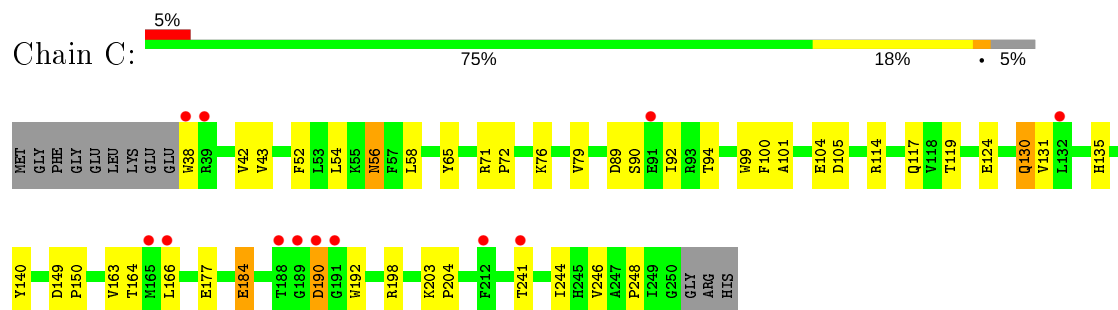
• Molecule 1: Predicted protein



• Molecule 1: Predicted protein

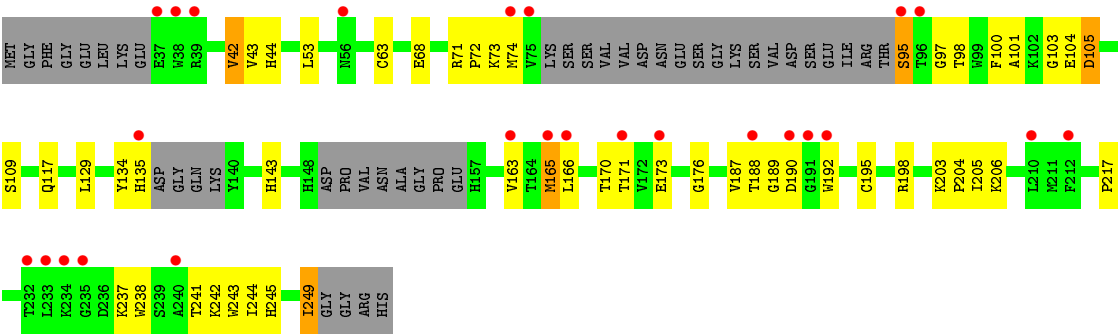


• Molecule 1: Predicted protein

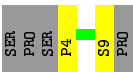
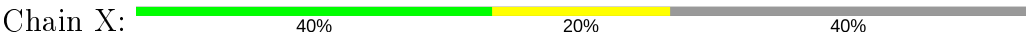


• Molecule 1: Predicted protein





● Molecule 2: Peptide substrate (Ser-Pro)5



● Molecule 2: Peptide substrate (Ser-Pro)5



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.25Å 58.75Å 105.16Å 90.00° 102.21° 90.00°	Depositor
Resolution (Å)	20.60 – 1.98 24.49 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.60-1.98) 93.4 (24.49-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 1.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.217 , 0.254 0.219 , 0.254	Depositor DCC
R_{free} test set	3435 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6949	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.87% 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: ZN, 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	1.00	1/1752 (0.1%)	0.96	0/2375
1	B	0.92	0/1545	0.94	0/2091
1	C	0.89	0/1747	0.93	0/2369
1	D	0.89	0/1498	0.94	0/2028
2	X	1.15	0/41	1.27	0/56
2	Y	0.82	0/55	1.05	0/76
All	All	0.93	1/6638 (0.0%)	0.95	0/8995

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	179	VAL	CB-CG1	5.04	1.63	1.52

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	1699	0	1653	19	0
1	B	1496	0	1466	36	0
1	C	1702	0	1643	39	0
1	D	1459	0	1416	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	X	39	0	36	3	0
2	Y	52	0	48	4	0
3	A	5	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	3	0	0
4	B	8	0	6	0	0
4	C	4	0	3	0	0
4	D	4	0	3	1	0
5	A	152	0	0	3	1
5	B	108	0	0	4	0
5	C	127	0	0	6	0
5	D	74	0	0	3	0
5	X	3	0	0	0	0
5	Y	4	0	0	0	0
All	All	6949	0	6277	131	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 10.

The worst 5 of 131 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:C:38:TRP:N	1:C:117[B]:GLN:HE22	1.49	1.11
1:D:176:GLY:O	1:D:237:LYS:NZ	2.10	0.83
1:A:92:ILE:HG21	2:X:4:PRO:HD2	1.61	0.83
1:B:56:ASN:OD1	5:B:366:HOH:O	2.02	0.78
1:B:149:ASP:HA	1:B:150:PRO:C	2.06	0.76

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)
5:A:15:HOH:O	5:A:437:HOH:O[2_555]	2.06	0.14

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	216/225 (96%)	214 (99%)	2 (1%)	0	100	100
1	B	182/225 (81%)	180 (99%)	2 (1%)	0	100	100
1	C	215/225 (96%)	209 (97%)	6 (3%)	0	100	100
1	D	176/225 (78%)	174 (99%)	2 (1%)	0	100	100
2	X	4/10 (40%)	4 (100%)	0	0	100	100
2	Y	6/10 (60%)	6 (100%)	0	0	100	100
All	All	799/920 (87%)	787 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	187/191 (98%)	180 (96%)	7 (4%)	34	22
1	B	163/191 (85%)	154 (94%)	9 (6%)	21	10
1	C	186/191 (97%)	179 (96%)	7 (4%)	33	21
1	D	158/191 (83%)	151 (96%)	7 (4%)	28	16
2	X	6/10 (60%)	6 (100%)	0	100	100
2	Y	8/10 (80%)	7 (88%)	1 (12%)	4	1
All	All	708/784 (90%)	677 (96%)	31 (4%)	29	16

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	190	ASP
1	C	130	GLN
1	D	242	LYS
1	B	194	GLU
1	C	135	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	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](#)

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](#)

Of 19 ligands modelled in this entry, 14 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	ACY	D	254	3	1,3,3	2.56	1 (100%)	0,3,3	0.00	-
4	ACY	C	254	3	1,3,3	0.93	0	0,3,3	0.00	-
4	ACY	B	5	3	1,3,3	0.65	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ACY	B	254	3	1,3,3	1.59	0	0,3,3	0.00	-
4	ACY	A	254	3	1,3,3	1.22	0	0,3,3	0.00	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	254	ACY	CH3-C	2.56	1.52	1.48

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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	254	ACY	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 [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	213/225 (94%)	0.18	10 (4%) 31 33	6, 11, 24, 34	0
1	B	186/225 (82%)	0.50	17 (9%) 9 10	6, 13, 26, 33	0
1	C	213/225 (94%)	0.25	12 (5%) 24 26	6, 12, 26, 33	0
1	D	182/225 (80%)	0.70	25 (13%) 3 3	5, 15, 26, 40	0
2	X	6/10 (60%)	-0.15	0 100 100	9, 11, 16, 23	0
2	Y	8/10 (80%)	0.41	0 100 100	11, 15, 24, 28	0
All	All	808/920 (87%)	0.39	64 (7%) 12 14	5, 12, 26, 40	0

The worst 5 of 64 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	75	VAL	9.2
1	B	75	VAL	8.8
1	A	166[A]	LEU	5.6
1	B	191	GLY	5.1
1	A	190	ASP	4.9

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. 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
3	ZN	B	14	1/1	0.91	0.06	31,31,31,31	0
4	ACY	D	254	4/4	0.96	0.17	17,18,18,20	0
4	ACY	B	254	4/4	0.97	0.12	12,13,13,15	0
4	ACY	B	5	4/4	0.97	0.07	6,7,8,8	0
3	ZN	B	12	1/1	0.97	0.03	46,46,46,46	0
4	ACY	A	254	4/4	0.97	0.16	8,8,8,11	0
3	ZN	A	8	1/1	0.97	0.06	36,36,36,36	0
4	ACY	C	254	4/4	0.97	0.12	9,9,10,10	0
3	ZN	A	10	1/1	0.97	0.06	29,29,29,29	1
3	ZN	D	13	1/1	0.98	0.07	54,54,54,54	0
3	ZN	C	9	1/1	0.98	0.06	33,33,33,33	1
3	ZN	C	6	1/1	0.99	0.05	15,15,15,15	0
3	ZN	C	11	1/1	0.99	0.03	29,29,29,29	1
3	ZN	A	5	1/1	1.00	0.06	12,12,12,12	0
3	ZN	A	7	1/1	1.00	0.03	9,9,9,9	1
3	ZN	B	2	1/1	1.00	0.08	10,10,10,10	0
3	ZN	A	1	1/1	1.00	0.09	9,9,9,9	0
3	ZN	D	4	1/1	1.00	0.08	10,10,10,10	0
3	ZN	C	3	1/1	1.00	0.08	10,10,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.