



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:02 AM GMT

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

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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

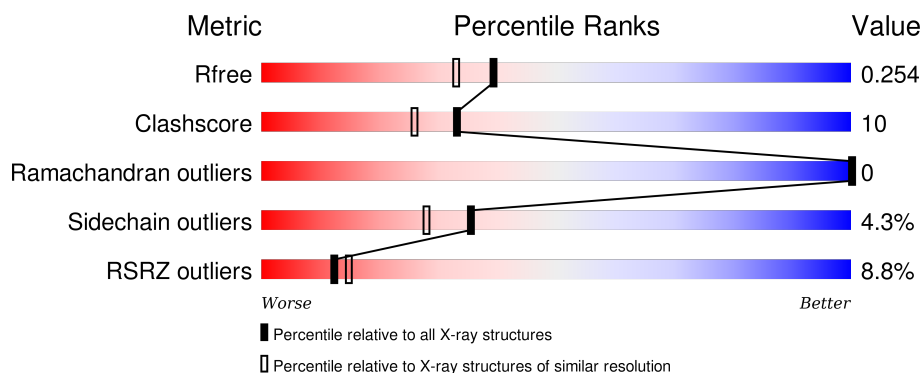
# 1 Overall quality at a glance

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))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (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  $\geq 3$ , 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	225	<div> <div>5%</div> <div>80% 15% 5%</div> </div>
1	B	225	<div> <div>8%</div> <div>65% 16% 17%</div> </div>
1	C	225	<div> <div>6%</div> <div>75% 18% 5%</div> </div>
1	D	225	<div> <div>12%</div> <div>58% 20% 19%</div> </div>
2	X	10	<div> <div>40% 20% 40%</div> </div>

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Mol	Chain	Length	Quality of chain
2	Y	10	 A horizontal bar chart showing the quality of chain Y. The bar is divided into four segments: 50% green, 20% yellow, 10% orange, and 20% grey. The percentages are labeled below the bar.

## 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

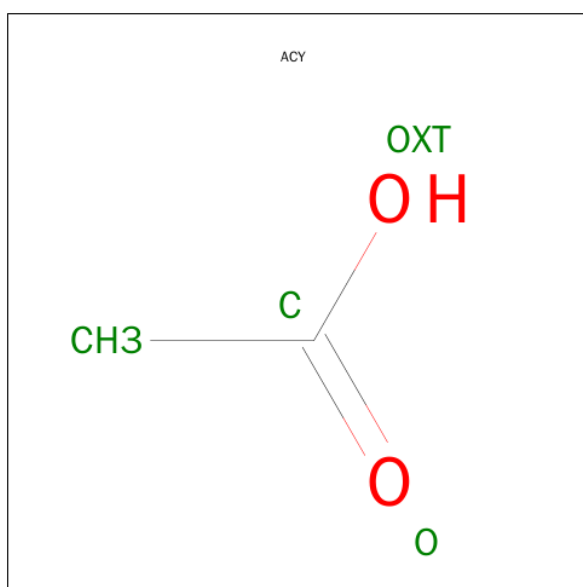
- Molecule 2 is a protein called Peptide substrate (Ser-Pro)5.

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 3	Zn 3	0	0
3	A	5	Total 5	Zn 5	0	0
3	D	2	Total 2	Zn 2	0	0
3	C	4	Total 4	Zn 4	0	0

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

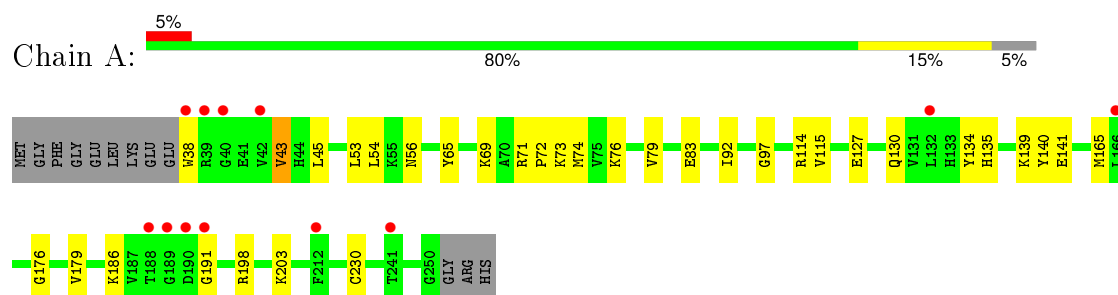
- Molecule 5 is water.

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

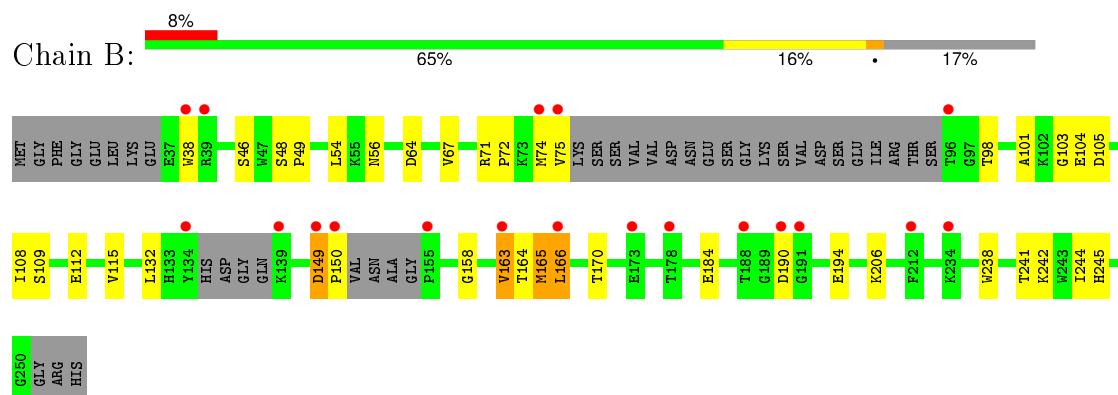
### 3 Residue-property plots [i](#)

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

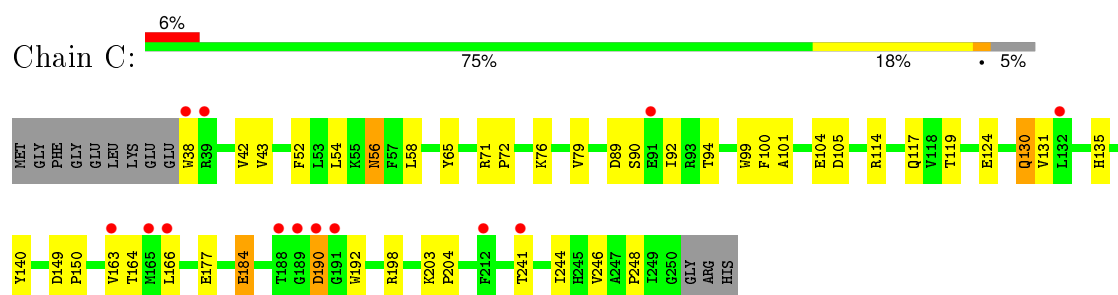
- Molecule 1: Predicted protein



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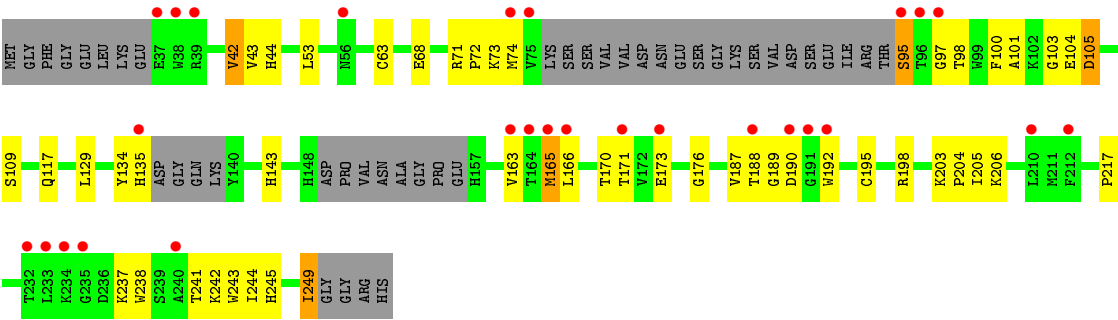


- Molecule 1: Predicted protein

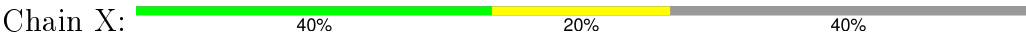


- Molecule 1: Predicted protein

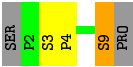




• Molecule 2: Peptide substrate (Ser-Pro)5



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.63 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, $R_{free}$	0.217 , 0.254 0.219 , 0.254	Depositor DCC
$R_{free}$ test set	3434 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 57.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 68688 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6949	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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.

All (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
1:B:166:LEU:HD12	1:B:241:THR:HG22	1.66	0.75
1:D:117:GLN:OE1	5:D:288:HOH:O	2.06	0.74
1:B:163[A]:VAL:HG12	1:B:244:ILE:HB	1.70	0.73
1:A:83:GLU:OE2	5:A:311:HOH:O	2.06	0.73
1:C:38:TRP:N	1:C:117[B]:GLN:NE2	2.33	0.72
1:C:56:ASN:OD1	5:C:466:HOH:O	2.07	0.72
1:B:115:VAL:HG13	1:B:165:MET:HE3	1.71	0.71
1:A:92:ILE:HD11	5:A:291:HOH:O	1.91	0.70
2:Y:3:SER:HB3	2:Y:4:PRO:HD2	1.74	0.69
1:B:149:ASP:CA	1:B:150:PRO:C	2.61	0.69
1:D:188:THR:HG22	1:D:189:GLY:N	2.06	0.69
1:C:92:ILE:C	1:C:92:ILE:HD12	2.12	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLU:OE2	5:B:332:HOH:O	2.10	0.69
1:C:184:GLU:OE2	5:C:344:HOH:O	2.10	0.69
1:C:101:ALA:HB3	1:C:104:GLU:OE1	1.93	0.69
1:B:149:ASP:HB2	1:B:150:PRO:HA	1.74	0.69
1:A:43:VAL:HG13	1:A:53:LEU:HB3	1.76	0.67
1:B:132:LEU:HG	5:B:312:HOH:O	1.94	0.66
1:C:163[A]:VAL:HG13	1:C:244:ILE:HD12	1.77	0.66
1:C:42:VAL:CG1	1:C:43:VAL:N	2.59	0.65
1:B:166:LEU:HD12	1:B:241:THR:CG2	2.27	0.63
1:B:149:ASP:HB2	1:B:150:PRO:CA	2.30	0.62
1:A:115:VAL:HG13	1:A:165:MET:HE3	1.82	0.61
1:B:150:PRO:HB3	1:D:243:TRP:CH2	2.36	0.61
1:D:95:SER:HB2	1:D:135:HIS:H	1.66	0.61
1:D:188:THR:CG2	1:D:189:GLY:N	2.64	0.60
1:D:173:GLU:HB2	5:D:281:HOH:O	2.02	0.60
1:C:42:VAL:HG12	1:C:43:VAL:N	2.16	0.60
1:B:150:PRO:HB3	1:D:243:TRP:CZ2	2.37	0.59
1:B:241:THR:HG23	5:B:312:HOH:O	2.01	0.59
1:B:149:ASP:CB	1:B:150:PRO:CA	2.80	0.59
1:A:127:GLU:HB3	2:X:9:SER:HB2	1.85	0.58
1:D:245:HIS:CD2	1:D:249:ILE:HD11	2.38	0.58
1:B:64:ASP:OD1	1:B:206:LYS:NZ	2.33	0.58
1:B:74:MET:SD	1:B:98:THR:HG22	2.43	0.57
1:C:42:VAL:CG1	1:C:43:VAL:H	2.16	0.57
1:C:100:PHE:HE2	1:C:131:VAL:HG21	1.70	0.56
1:D:170:THR:HG23	1:D:238:TRP:HB2	1.88	0.56
1:C:90:SER:OG	1:C:92:ILE:HG13	2.04	0.56
1:B:103:GLY:HA2	1:B:109:SER:OG	2.05	0.56
1:B:149:ASP:CB	1:B:150:PRO:C	2.75	0.55
1:A:191:GLY:O	1:A:203:LYS:HE2	2.07	0.55
1:A:54:LEU:HD12	1:A:54:LEU:N	2.22	0.55
1:D:166:LEU:HD11	4:D:254:ACY:H2	1.89	0.55
1:D:43:VAL:HB	1:D:53:LEU:HB3	1.89	0.54
1:D:74:MET:SD	1:D:98:THR:HG22	2.47	0.54
1:A:79:VAL:HG21	2:X:4:PRO:HG3	1.89	0.54
1:C:117[B]:GLN:NE2	5:C:401:HOH:O	2.39	0.54
1:D:171:THR:HA	1:D:204:PRO:O	2.07	0.54
1:C:192:TRP:CZ3	1:C:203:LYS:HG2	2.43	0.54
1:D:68:GLU:OE1	1:D:68:GLU:HA	2.09	0.53
1:B:38:TRP:CH2	1:B:54:LEU:HD23	2.44	0.53
1:D:166:LEU:HD12	1:D:241:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:CYS:O	1:D:198:ARG:HG3	2.09	0.52
1:C:71:ARG:HB2	1:C:72:PRO:HD3	1.91	0.52
1:B:48:SER:HB3	1:B:184:GLU:HG3	1.91	0.52
1:B:67:VAL:O	1:B:71:ARG:HG3	2.10	0.52
1:A:186:LYS:NZ	1:A:198:ARG:O	2.36	0.52
1:C:100:PHE:CE2	1:C:131:VAL:HG21	2.45	0.51
1:D:103:GLY:HA2	1:D:109:SER:OG	2.10	0.51
1:C:42:VAL:HG13	1:C:43:VAL:H	1.76	0.51
1:D:100:PHE:HD2	1:D:129:LEU:HD23	1.76	0.50
1:D:95:SER:CB	1:D:135:HIS:H	2.23	0.50
1:A:76:LYS:NZ	5:A:432:HOH:O	2.44	0.50
1:D:163[A]:VAL:CG1	1:D:244:ILE:HB	2.42	0.49
1:B:38:TRP:CZ3	1:B:54:LEU:HD23	2.47	0.49
1:C:124:GLU:HB3	1:C:248:PRO:HB3	1.94	0.49
1:D:105:ASP:C	1:D:105:ASP:OD1	2.50	0.49
1:D:134:TYR:HB2	1:D:237:LYS:HB3	1.95	0.49
1:D:163[A]:VAL:HG12	1:D:244:ILE:HB	1.94	0.49
1:C:54:LEU:N	1:C:54:LEU:HD12	2.28	0.49
1:D:101:ALA:HB3	1:D:104:GLU:HB2	1.94	0.48
1:C:79:VAL:HG21	2:Y:4:PRO:HG2	1.95	0.48
1:B:158:GLY:O	1:B:245:HIS:HB3	2.14	0.48
1:C:76:LYS:HE3	1:C:94:THR:HA	1.94	0.48
1:B:101:ALA:O	1:B:104:GLU:HB3	2.13	0.48
1:C:52:PHE:N	1:C:52:PHE:CD1	2.82	0.48
1:C:163[B]:VAL:HG12	1:C:164:THR:N	2.29	0.47
1:B:71:ARG:HB2	1:B:72:PRO:CD	2.44	0.47
1:C:190:ASP:OD1	1:C:190:ASP:N	2.44	0.47
1:B:163[A]:VAL:HG13	1:B:244:ILE:HD12	1.96	0.47
1:C:119:THR:HG21	1:C:244:ILE:CD1	2.45	0.47
1:C:130:GLN:HB3	1:C:241:THR:OG1	2.15	0.47
1:A:176:GLY:HA2	1:A:230:CYS:O	2.14	0.46
1:A:65:TYR:CZ	1:A:69:LYS:HE3	2.50	0.46
1:C:149:ASP:HB2	1:C:150:PRO:HD2	1.96	0.46
1:B:115:VAL:HG13	1:B:165:MET:CE	2.41	0.46
1:A:74:MET:HE1	1:A:97:GLY:HA2	1.98	0.46
1:C:246:VAL:O	1:D:217:PRO:HB2	2.17	0.45
1:C:54:LEU:N	1:C:54:LEU:CD1	2.80	0.45
1:C:117[A]:GLN:OE1	1:D:44:HIS:HB2	2.16	0.45
1:D:166:LEU:HA	1:D:241:THR:HG22	1.99	0.45
1:C:65:TYR:OH	1:C:105:ASP:OD2	2.19	0.45
5:C:402:HOH:O	1:D:42:VAL:HG11	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:VAL:HG21	2:Y:4:PRO:CG	2.46	0.44
1:C:99:TRP:CZ3	2:Y:9:SER:HA	2.52	0.44
1:C:71:ARG:CB	1:C:72:PRO:HD3	2.47	0.44
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.82	0.44
1:B:74:MET:SD	1:B:98:THR:CG2	3.06	0.44
1:A:71:ARG:HB2	1:A:72:PRO:HD3	2.00	0.43
1:B:46[B]:SER:OG	1:B:49:PRO:O	2.22	0.43
1:C:177:GLU:HA	1:C:204:PRO:HD3	1.99	0.43
1:B:164:THR:HG22	1:B:166:LEU:HD13	2.00	0.43
1:C:76:LYS:HD3	1:C:89:ASP:OD1	2.19	0.42
1:C:203:LYS:HE2	5:C:448:HOH:O	2.19	0.42
1:A:139:LYS:HE3	1:A:141:GLU:HG3	2.01	0.42
1:D:205:ILE:O	1:D:206:LYS:C	2.58	0.42
1:D:63:CYS:HB2	1:D:206:LYS:HE3	2.00	0.42
1:B:150:PRO:HD3	1:D:143:HIS:CD2	2.55	0.42
1:D:165:MET:HE3	1:D:165:MET:HB3	1.88	0.41
1:A:54:LEU:N	1:A:54:LEU:CD1	2.83	0.41
1:D:73:LYS:HE2	1:D:73:LYS:HB3	1.86	0.41
1:C:198:ARG:HB2	5:C:272:HOH:O	2.20	0.41
1:B:108:ILE:O	1:B:112:GLU:HG3	2.21	0.41
1:D:71:ARG:HB3	1:D:72:PRO:HD3	2.02	0.41
1:D:74:MET:CE	1:D:97:GLY:HA2	2.50	0.41
1:B:170:THR:HG23	1:B:238:TRP:HB2	2.02	0.41
1:A:38:TRP:HB2	1:A:114:ARG:HD3	2.02	0.41
1:D:249:ILE:HD12	1:D:249:ILE:HA	1.78	0.40
1:D:187:VAL:HG21	1:D:192:TRP:CD2	2.56	0.40
1:B:163[A]:VAL:CG1	1:B:244:ILE:HB	2.44	0.40
1:D:188:THR:CG2	1:D:189:GLY:H	2.33	0.40
1:C:58:LEU:HD23	1:C:114:ARG:NH1	2.36	0.40
1:D:173:GLU:CB	5:D:281:HOH:O	2.64	0.40
1:B:242:LYS:HA	1:B:242:LYS:HD3	1.89	0.40
1:D:203:LYS:HB3	1:D:203:LYS:HE3	1.87	0.40

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%)	41	35
1	B	163/191 (85%)	154 (94%)	9 (6%)	27	18
1	C	186/191 (97%)	179 (96%)	7 (4%)	40	33
1	D	158/191 (83%)	151 (96%)	7 (4%)	35	27
2	X	6/10 (60%)	6 (100%)	0	100	100
2	Y	8/10 (80%)	7 (88%)	1 (12%)	6	2
All	All	708/784 (90%)	677 (96%)	31 (4%)	35	27

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	VAL
1	A	56	ASN
1	A	73	LYS
1	A	130	GLN
1	A	134	TYR
1	A	135	HIS
1	A	140	TYR
1	B	75	VAL
1	B	105	ASP
1	B	149	ASP
1	B	163[A]	VAL
1	B	163[B]	VAL
1	B	165	MET
1	B	166	LEU
1	B	190	ASP
1	B	194	GLU
1	C	56	ASN
1	C	130	GLN
1	C	135	HIS
1	C	140	TYR
1	C	166	LEU
1	C	184	GLU
1	C	190	ASP
1	D	42	VAL
1	D	95	SER
1	D	105	ASP
1	D	165	MET
1	D	190	ASP
1	D	242	LYS
1	D	249	ILE
2	Y	9	SER

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 ⓘ

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	A	254	3	1,3,3	1.06	0	0,3,3	0.00	-
4	ACY	B	254	3	1,3,3	1.40	0	0,3,3	0.00	-
4	ACY	B	5	3	1,3,3	0.53	0	0,3,3	0.00	-
4	ACY	C	254	3	1,3,3	0.92	0	0,3,3	0.00	-
4	ACY	D	254	3	1,3,3	2.29	1 (100%)	0,3,3	0.00	-

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	ACY	A	254	3	-	0/0/0/0	0/0/0/0
4	ACY	B	254	3	-	0/0/0/0	0/0/0/0
4	ACY	B	5	3	-	0/0/0/0	0/0/0/0
4	ACY	C	254	3	-	0/0/0/0	0/0/0/0
4	ACY	D	254	3	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	254	ACY	CH3-C	2.29	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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	213/225 (94%)	0.22	12 (5%) 28 32	6, 11, 24, 34	0
1	B	186/225 (82%)	0.54	19 (10%) 9 11	6, 13, 26, 33	0
1	C	213/225 (94%)	0.29	13 (6%) 25 28	6, 12, 26, 33	0
1	D	182/225 (80%)	0.74	27 (14%) 3 4	5, 15, 26, 40	0
2	X	6/10 (60%)	-0.11	0 100 100	9, 11, 16, 23	0
2	Y	8/10 (80%)	0.46	0 100 100	11, 15, 24, 28	0
All	All	808/920 (87%)	0.43	71 (8%) 12 15	5, 12, 26, 40	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	75	VAL	9.5
1	B	75	VAL	9.1
1	A	166[A]	LEU	5.8
1	B	191	GLY	5.1
1	A	190	ASP	5.0
1	D	190	ASP	4.8
1	D	233	LEU	4.7
1	D	95	SER	4.4
1	C	38	TRP	4.4
1	C	190	ASP	4.3
1	C	189	GLY	3.9
1	C	39	ARG	3.9
1	A	189	GLY	3.8
1	D	38	TRP	3.6
1	B	96	THR	3.4
1	B	166	LEU	3.4
1	A	188	THR	3.3
1	D	188	THR	3.3
1	D	39	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	166	LEU	3.2
1	B	155	PRO	3.2
1	C	166	LEU	3.2
1	A	39	ARG	3.2
1	B	188	THR	2.9
1	A	191	GLY	2.9
1	B	149	ASP	2.9
1	D	96	THR	2.9
1	D	232	THR	2.9
1	B	190	ASP	2.8
1	D	191	GLY	2.8
1	D	37	GLU	2.8
1	D	56	ASN	2.8
1	D	240	ALA	2.7
1	C	91	GLU	2.7
1	A	38	TRP	2.7
1	C	188	THR	2.6
1	D	192	TRP	2.6
1	D	171	THR	2.6
1	D	165	MET	2.5
1	D	74	MET	2.5
1	D	210	LEU	2.5
1	D	173	GLU	2.4
1	B	39	ARG	2.4
1	C	241	THR	2.4
1	B	139	LYS	2.4
1	B	163[A]	VAL	2.4
1	B	173	GLU	2.4
1	D	234	LYS	2.4
1	D	163[A]	VAL	2.4
1	A	212	PHE	2.4
1	C	132	LEU	2.3
1	D	135	HIS	2.3
1	B	150	PRO	2.3
1	B	134	TYR	2.3
1	B	234	LYS	2.2
1	D	235	GLY	2.2
1	A	241	THR	2.2
1	C	212	PHE	2.2
1	B	38	TRP	2.2
1	C	191	GLY	2.2
1	A	132	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	212	PHE	2.1
1	B	212	PHE	2.1
1	B	178	THR	2.1
1	B	74	MET	2.1
1	D	97	GLY	2.1
1	A	42	VAL	2.1
1	A	40	GLY	2.0
1	C	163[A]	VAL	2.0
1	D	164	THR	2.0
1	C	165	MET	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	ACY	D	254	4/4	0.96	0.17	0.50	17,18,18,20	0
4	ACY	A	254	4/4	0.97	0.16	-0.09	8,8,8,11	0
4	ACY	B	254	4/4	0.97	0.12	-0.26	12,13,13,15	0
3	ZN	A	1	1/1	1.00	0.09	-0.42	9,9,9,9	0
4	ACY	C	254	4/4	0.97	0.12	-0.52	9,9,10,10	0
3	ZN	D	4	1/1	1.00	0.08	-0.95	10,10,10,10	0
3	ZN	C	3	1/1	1.00	0.08	-1.13	10,10,10,10	0
4	ACY	B	5	4/4	0.97	0.07	-1.79	6,7,8,8	0
3	ZN	C	9	1/1	0.98	0.06	-	33,33,33,33	1
3	ZN	B	2	1/1	1.00	0.08	-	10,10,10,10	0
3	ZN	A	10	1/1	0.97	0.06	-	29,29,29,29	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	12	1/1	0.97	0.03	-	46,46,46,46	0
3	ZN	A	7	1/1	1.00	0.03	-	9,9,9,9	1
3	ZN	A	5	1/1	1.00	0.06	-	12,12,12,12	0
3	ZN	A	8	1/1	0.97	0.06	-	36,36,36,36	0
3	ZN	C	11	1/1	0.99	0.03	-	29,29,29,29	1
3	ZN	D	13	1/1	0.98	0.07	-	54,54,54,54	0
3	ZN	C	6	1/1	0.99	0.06	-	15,15,15,15	0
3	ZN	B	14	1/1	0.91	0.06	-	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.