



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:58 PM UTC

PDB ID : 3GZE / pdb_00003gze
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 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

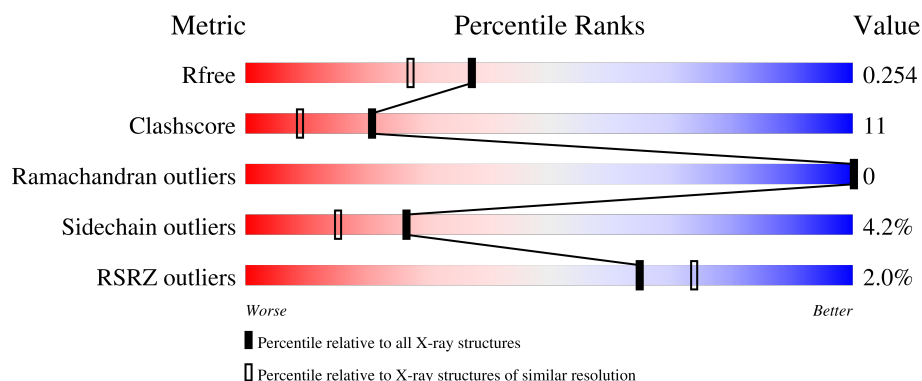
1 Overall quality at a glance

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}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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 $\leq 5\%$. 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	79% 15% • 5%
1	B	225	2% 64% 16% • 17%
1	C	225	72% 20% • 5%
1	D	225	3% 57% 20% • 19%
2	X	10	40% 20% 40%

Continued on next page...

Continued from previous page...

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

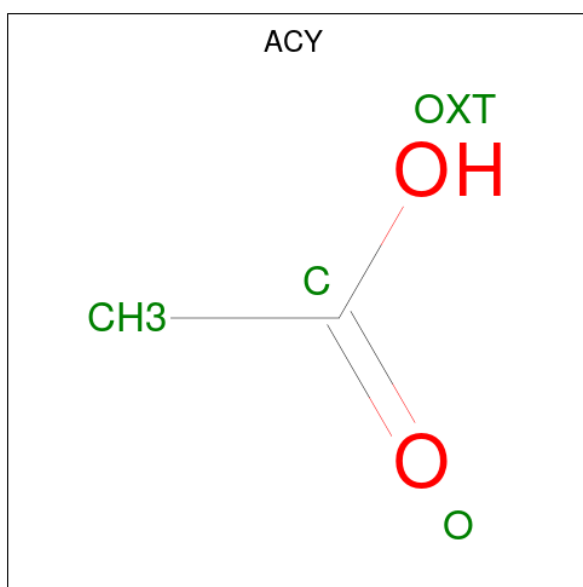
- Molecule 2 is a protein called Peptide substrate (Ser-Pro)5.

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is ACETIC ACID (CCD ID: 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		

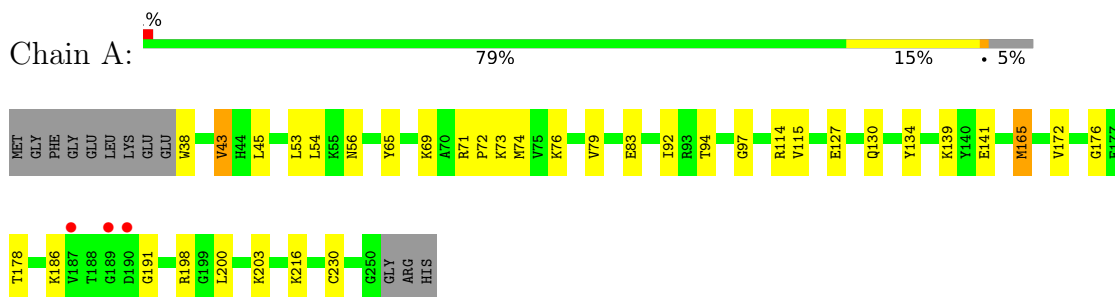
- Molecule 5 is water.

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

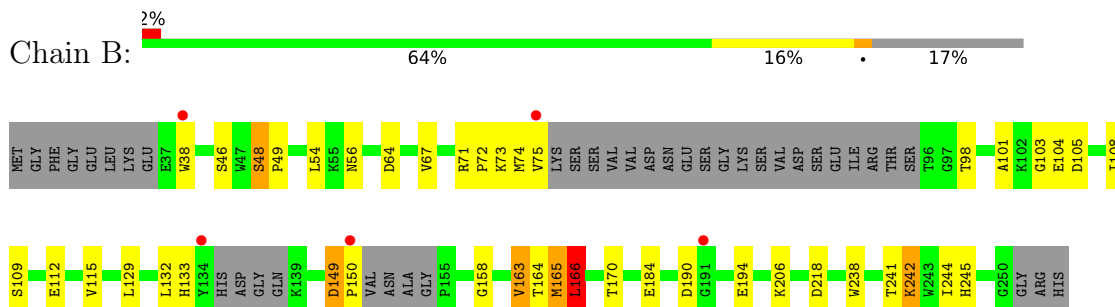
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

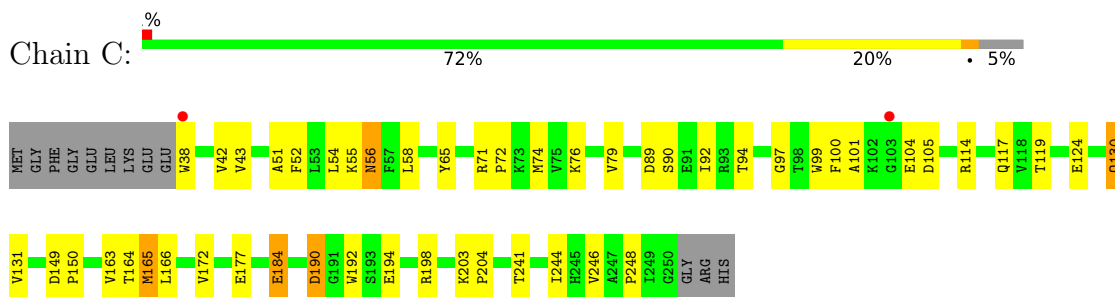
• Molecule 1: Predicted protein



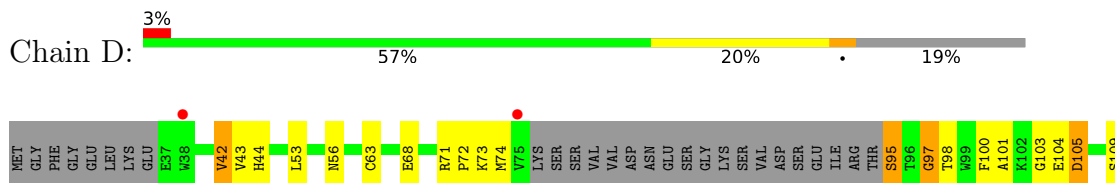
• Molecule 1: Predicted protein

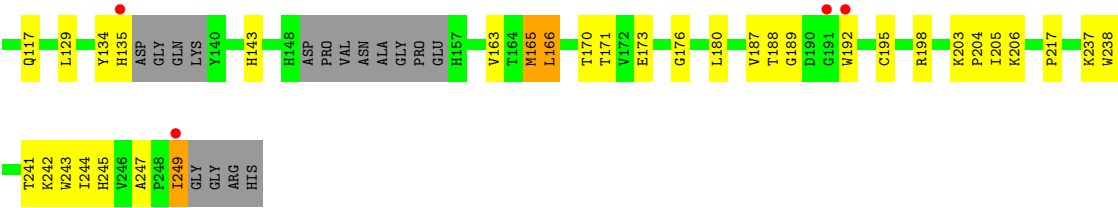


• Molecule 1: Predicted protein

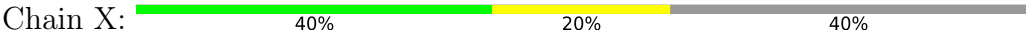


• Molecule 1: Predicted protein





● 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 20.60 – 1.98	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.60-1.98) 93.4 (20.60-1.98)	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 0.220 , 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)	0.42 , 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	0.91	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, ZN

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	1.27	2/1752 (0.1%)	1.17	4/2375 (0.2%)
1	B	1.18	3/1545 (0.2%)	1.15	0/2091
1	C	1.14	0/1747	1.14	2/2369 (0.1%)
1	D	1.15	1/1498 (0.1%)	1.18	3/2028 (0.1%)
2	X	1.47	0/41	1.65	0/56
2	Y	1.08	0/55	1.28	0/76
All	All	1.19	6/6638 (0.1%)	1.16	9/8995 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	247	ALA	N-CA	7.79	1.51	1.46
1	A	172	VAL	CA-CB	5.82	1.61	1.54
1	B	166	LEU	C-O	-5.58	1.17	1.24
1	B	129	LEU	CA-C	-5.38	1.46	1.52
1	B	48	SER	C-O	-5.25	1.19	1.24
1	A	94	THR	C-O	-5.07	1.16	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	LYS	CA-C-N	-6.41	113.21	119.87
1	A	216	LYS	C-N-CA	-6.41	113.21	119.87
1	D	180	LEU	CA-C-N	6.27	125.83	119.19
1	D	180	LEU	C-N-CA	6.27	125.83	119.19
1	D	97	GLY	N-CA-C	5.99	119.53	110.18
1	C	194	GLU	N-CA-C	-5.73	105.18	111.82
1	A	200	LEU	N-CA-C	-5.46	102.21	110.28
1	C	172	VAL	N-CA-C	5.20	116.06	108.58
1	A	178	THR	N-CA-C	-5.02	101.58	109.25

There are no chirality outliers.

There are no planarity outliers.

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	1699	0	1653	20	0
1	B	1496	0	1466	41	0
1	C	1702	0	1643	43	0
1	D	1459	0	1416	42	0
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	7	0
5	D	74	0	0	4	0
5	X	3	0	0	0	0
5	Y	4	0	0	0	0
All	All	6949	0	6277	142	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 11.

All (142) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ASP:HA	1:B:150:PRO:C	2.06	0.81
1:B:115:VAL:HG13	1:B:165:MET:HE3	1.61	0.80
1:B:56:ASN:OD1	5:B:366:HOH:O	2.02	0.78
1:B:166:LEU:HD12	1:B:241:THR:HG22	1.66	0.75
1:B:149:ASP:CA	1:B:150:PRO:C	2.61	0.74
1:C:92:ILE:C	1:C:92:ILE:HD12	2.12	0.74
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: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:D:188:THR:HG22	1:D:189:GLY:N	2.06	0.69
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:C:54:LEU:HD22	1:C:165:MET:HE1	1.81	0.62
1:B:74:MET:HE2	1:B:133:HIS:HB2	1.81	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:B:149:ASP:CB	1:B:150:PRO:C	2.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:THR:HG23	1:D:238:TRP:HB2	1.88	0.56
1:B:103:GLY:HA2	1:B:109:SER:OG	2.05	0.56
1:C:90:SER:OG	1:C:92:ILE:HG13	2.04	0.56
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:105:ASP:OD1	1:D:105:ASP:C	2.50	0.54
1:B:74:MET:HE2	1:B:133:HIS:CB	2.37	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:HA	1:D:68:GLU:OE1	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
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:A:115:VAL:HG13	1:A:165:MET:HE3	1.91	0.52
1:A:186:LYS:NZ	1:A:198:ARG:O	2.36	0.52
1:B:67:VAL:O	1:B:71:ARG:HG3	2.10	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: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:HD12	1:C:54:LEU:N	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:CD1	1:C:52:PHE:N	2.82	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:205:ILE:O	1:D:206:LYS:C	2.58	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:C:163[B]:VAL:HG12	1:C:164:THR:N	2.29	0.46
1:A:165:MET:HB2	1:A:165:MET:HE2	1.68	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
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:A:74:MET:HE1	1:A:97:GLY:HA2	1.99	0.44
1:A:45:LEU:HD23	1:A:45:LEU:HA	1.82	0.44
1:C:71:ARG:CB	1:C:72:PRO:HD3	2.47	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:C:55:LYS:NZ	5:C:327:HOH:O	2.51	0.43
1:B:46[B]:SER:OG	1:B:49:PRO:O	2.22	0.43
1:C:51:ALA:C	1:C:52:PHE:CD1	2.97	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: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:B:71:ARG:C	1:B:73:LYS:H	2.27	0.41
1:B:149:ASP:HB3	1:B:150:PRO:C	2.43	0.41
1:D:165:MET:HB3	1:D:165:MET:HE3	1.69	0.41
1:A:54:LEU:N	1:A:54:LEU:CD1	2.83	0.41
1:B:165:MET:HE2	1:B:165:MET:HB2	1.91	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:O	1:B:112:GLU:HG3	2.21	0.41
1:B:218:ASP:OD1	1:B:218:ASP:C	2.64	0.41
1:D:71:ARG:HB3	1:D:72:PRO:HD3	2.02	0.41
1:A:38:TRP:HB2	1:A:114:ARG:HD3	2.02	0.41
1:B:170:THR:HG23	1:B:238:TRP:HB2	2.02	0.41
1:D:74:MET:CE	1:D:97:GLY:HA2	2.50	0.41
1:D:187:VAL:HG21	1:D:192:TRP:CD2	2.56	0.40
1:D:249:ILE:HD12	1:D:249:ILE:HA	1.78	0.40
1:B:163[A]:VAL:CG1	1:B:244:ILE:HB	2.44	0.40
1:C:74:MET:HE1	1:C:97:GLY:HA2	2.03	0.40
1:C:58:LEU:HD23	1:C:114:ARG:NH1	2.36	0.40
1:D:56:ASN:CG	5:D:350:HOH:O	2.64	0.40
1:D:188:THR:CG2	1:D:189:GLY:H	2.33	0.40
1:B:242:LYS:HA	1:B:242:LYS:HD3	1.89	0.40
1:D:173:GLU:CB	5:D:281:HOH:O	2.64	0.40
1:D:203:LYS:HE3	1:D:203:LYS:HB3	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 [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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	181 (97%)	6 (3%)	34	24
1	B	163/191 (85%)	153 (94%)	10 (6%)	17	7
1	C	186/191 (97%)	180 (97%)	6 (3%)	34	24
1	D	158/191 (83%)	151 (96%)	7 (4%)	25	14
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%)	678 (96%)	30 (4%)	26	15

All (30) 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	165	MET
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	166	LEU
1	B	190	ASP
1	B	194	GLU
1	B	242	LYS
1	C	56	ASN
1	C	130	GLN
1	C	165	MET
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	166	LEU
1	D	242	LYS
1	D	249	ILE
2	Y	9	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	ASN
1	A	130	GLN
1	D	56	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	3,3,3	0.60	0	3,3,3	1.73	2 (66%)
4	ACY	C	254	3	3,3,3	0.80	0	3,3,3	0.67	0
4	ACY	B	5	3	3,3,3	1.03	0	3,3,3	0.34	0
4	ACY	B	254	3	3,3,3	0.87	0	3,3,3	1.28	0
4	ACY	D	254	3	3,3,3	0.96	0	3,3,3	1.03	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	254	ACY	O-C-CH3	-2.19	113.54	122.53
4	A	254	ACY	OXT-C-CH3	2.02	123.53	115.05

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

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(Å ²)	Q<0.9
1	A	213/225 (94%)	-0.17	3 (1%) 73 81	6, 11, 23, 34	5 (2%)
1	B	186/225 (82%)	0.37	5 (2%) 56 66	5, 13, 26, 33	4 (2%)
1	C	213/225 (94%)	-0.13	2 (0%) 81 86	4, 12, 26, 33	4 (1%)
1	D	182/225 (80%)	0.32	6 (3%) 49 59	4, 15, 26, 40	2 (1%)
2	X	6/10 (60%)	-0.01	0 100 100	9, 11, 16, 23	0
2	Y	8/10 (80%)	-0.10	0 100 100	11, 15, 24, 28	0
All	All	808/920 (87%)	0.08	16 (1%) 65 74	4, 12, 26, 40	15 (1%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	75	VAL	3.9
1	D	75	VAL	3.7
1	D	38	TRP	3.5
1	A	190	ASP	3.0
1	C	38	TRP	3.0
1	B	150	PRO	2.8
1	B	38	TRP	2.7
1	B	191	GLY	2.7
1	B	134	TYR	2.7
1	D	192	TRP	2.4
1	A	187	VAL	2.2
1	D	135	HIS	2.1
1	D	191	GLY	2.1
1	D	249	ILE	2.1
1	A	189	GLY	2.0
1	C	103	GLY	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	ZN	B	14	1/1	0.87	0.08	31,31,31,31	0
3	ZN	D	13	1/1	0.93	0.07	54,54,54,54	0
4	ACY	D	254	4/4	0.95	0.12	17,18,18,20	0
3	ZN	C	11	1/1	0.96	0.04	29,29,29,29	1
3	ZN	B	12	1/1	0.96	0.05	46,46,46,46	0
3	ZN	A	10	1/1	0.96	0.06	29,29,29,29	1
3	ZN	C	9	1/1	0.97	0.04	33,33,33,33	1
4	ACY	A	254	4/4	0.97	0.05	8,8,8,11	0
4	ACY	C	254	4/4	0.97	0.06	9,9,10,10	0
3	ZN	A	8	1/1	0.97	0.07	36,36,36,36	0
3	ZN	C	6	1/1	0.98	0.04	15,15,15,15	0
4	ACY	B	254	4/4	0.98	0.06	12,13,13,15	0
3	ZN	D	4	1/1	0.99	0.06	10,10,10,10	0
4	ACY	B	5	4/4	0.99	0.05	6,7,8,8	0
3	ZN	A	7	1/1	0.99	0.02	9,9,9,9	1
3	ZN	A	5	1/1	0.99	0.01	12,12,12,12	0
3	ZN	B	2	1/1	1.00	0.04	10,10,10,10	0
3	ZN	C	3	1/1	1.00	0.01	10,10,10,10	0
3	ZN	A	1	1/1	1.00	0.03	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.