



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:15 PM GMT

PDB ID : 1WX5  
Title : Crystal Structure of the copper-free Streptomyces castaneoglobisporus tyrosinase complexed with a caddie protein in the monoclinic crystal  
Authors : Matoba, Y.; Kumagai, T.; Yamamoto, A.; Yoshitsu, H.; Sugiyama, M.  
Deposited on : 2005-01-19  
Resolution : 2.02 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

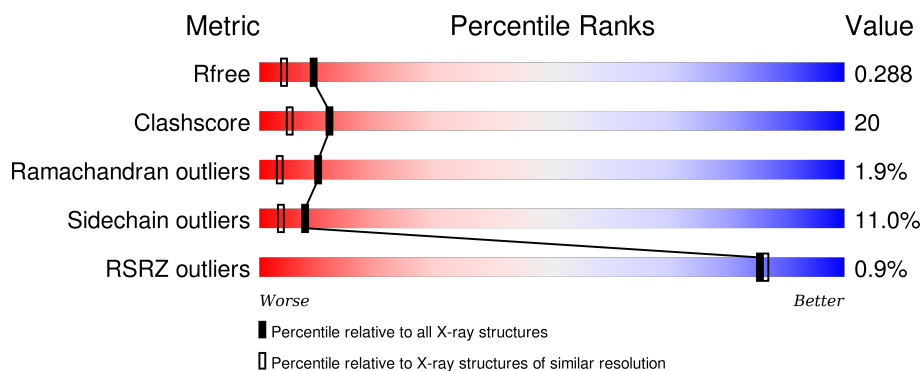
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	7858 (2.04-2.00)
Clashscore	102246	9060 (2.04-2.00)
Ramachandran outliers	100387	8952 (2.04-2.00)
Sidechain outliers	100360	8951 (2.04-2.00)
RSRZ outliers	91569	7873 (2.04-2.00)

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 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	281	<div> <div>58%</div> <div>36%</div> <div>• •</div> </div>
1	C	281	<div> <div>57%</div> <div>34%</div> <div>6% •</div> </div>
2	B	134	<div> <div>%</div> <div>29%</div> <div>20%</div> <div>•</div> <div>47%</div> </div>
2	D	134	<div> <div>3%</div> <div>19%</div> <div>32%</div> <div>•</div> <div>44%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	C	282	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6027 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 tyrosinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	S	0	0	0
			2212	1393	404	411	4			
1	C	273	Total	C	N	O	S	0	0	0
			2193	1382	400	407	4			

- Molecule 2 is a protein called MelC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C	N	O	S	0	0	0
			546	345	99	101	1			
2	D	75	Total	C	N	O	S	0	0	0
			573	360	105	107	1			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	C	2	Total	Na	0	0
			2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	221	Total	O	0	0
			221	221		

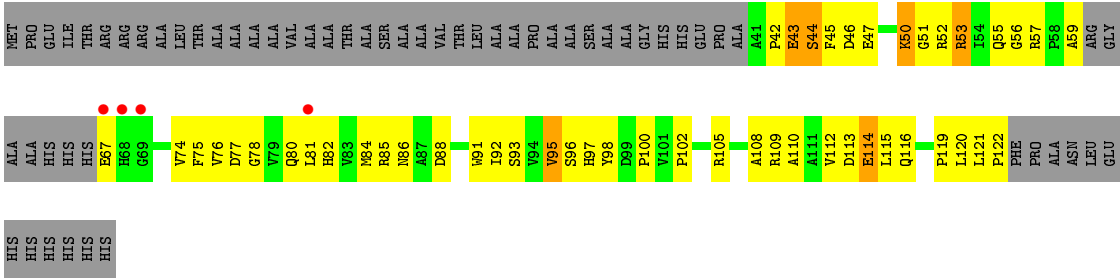
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	44	Total 44	O 44	0	0
5	C	192	Total 192	O 192	0	0
5	D	41	Total 41	O 41	0	0



● Molecule 2: MelC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.85Å 93.20Å 65.59Å 90.00° 93.80° 90.00°	Depositor
Resolution (Å)	30.00 – 2.02 40.69 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-2.02) 82.6 (40.69-2.02)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.201 , 0.291 0.200 , 0.288	Depositor DCC
$R_{free}$ test set	2301 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	15.1	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 23.1	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 46161 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.16% 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: NA, CL

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	0.36	0/2280	0.60	0/3113
1	C	0.35	0/2260	0.59	0/3086
2	B	0.32	0/560	0.54	0/763
2	D	0.31	0/588	0.52	0/800
All	All	0.35	0/5688	0.58	0/7762

There are no bond length outliers.

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	2212	0	2092	77	0
1	C	2193	0	2079	74	0
2	B	546	0	527	31	0
2	D	573	0	546	45	0
3	A	1	0	0	0	0
3	C	2	0	0	0	0
4	A	2	0	0	0	0
5	A	221	0	0	10	0
5	B	44	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	192	0	0	10	0
5	D	41	0	0	5	0
All	All	6027	0	5244	215	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 20.

All (215) 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:185:ARG:HH22	2:D:88:ASP:HB3	1.20	1.01
1:C:185:ARG:NH2	2:D:88:ASP:HB3	1.85	0.90
1:A:94:VAL:HG13	1:A:143:LEU:HD12	1.52	0.89
2:B:95:VAL:HG13	2:B:114:GLU:HG2	1.57	0.87
1:A:65:ARG:O	1:A:65:ARG:HD3	1.79	0.82
2:B:105:ARG:HH21	2:B:105:ARG:HG2	1.45	0.80
1:A:107:THR:HB	1:A:143:LEU:HG	1.62	0.80
1:A:27:ARG:HD2	5:A:482:HOH:O	1.83	0.78
1:A:30:ARG:NH2	1:A:76:SER:OG	2.23	0.71
1:C:157:GLU:HG2	5:C:305:HOH:O	1.89	0.71
2:B:95:VAL:CG1	2:B:114:GLU:HG2	2.21	0.71
1:C:109:ARG:HD3	1:C:116:MET:SD	2.31	0.70
2:D:81:LEU:HD11	2:D:93:SER:OG	1.91	0.70
1:A:245:VAL:HG11	1:A:251:MET:HG2	1.75	0.69
2:D:110:ALA:O	2:D:113:ASP:HB2	1.93	0.68
1:C:7:GLN:OE1	1:C:98:LEU:HB3	1.94	0.68
1:A:140:ARG:O	1:A:199:GLY:HA3	1.94	0.67
1:A:169:PRO:HG2	1:A:171:ASN:OD1	1.94	0.67
1:A:162:ILE:HG21	1:A:177:PHE:N	2.11	0.66
1:C:180:HIS:CD2	1:C:186:GLY:HA3	2.30	0.66
2:D:105:ARG:HD2	2:D:109:ARG:HH21	1.61	0.66
1:A:242:PRO:O	1:A:243:ASP:HB2	1.96	0.65
1:A:228:ARG:HE	1:A:274:LEU:HD13	1.62	0.65
1:A:157:GLU:HB3	5:A:344:HOH:O	1.97	0.65
2:D:74:VAL:HG11	2:D:81:LEU:HD23	1.80	0.64
1:C:107:THR:HB	1:C:143:LEU:HD12	1.78	0.64
2:B:105:ARG:HG2	2:B:105:ARG:NH2	2.12	0.64
1:A:132:ARG:HD2	1:A:136:ARG:O	1.99	0.63
1:C:129:ILE:HG12	1:C:137:THR:O	1.98	0.62
1:C:200:GLN:O	1:C:206:SER:HA	2.00	0.62
1:A:26:LYS:HE2	1:A:128:PRO:HD2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:LEU:HD21	1:C:73:ALA:O	1.99	0.61
1:C:95:ARG:HB3	5:C:465:HOH:O	1.99	0.61
2:D:95:VAL:O	2:D:95:VAL:HG13	1.99	0.61
2:B:46:ASP:HA	2:B:55:GLN:HB3	1.83	0.61
1:C:26:LYS:NZ	1:C:128:PRO:HD2	2.16	0.60
1:C:72:GLN:HG2	5:C:356:HOH:O	2.01	0.60
1:C:183:GLY:HA2	1:C:188:ASN:HA	1.83	0.60
2:D:108:ALA:O	2:D:112:VAL:HG23	2.02	0.59
2:B:82:HIS:HB2	5:B:152:HOH:O	2.01	0.59
2:D:85:ARG:HB2	2:D:91:TRP:CH2	2.37	0.59
1:A:13:ASP:OD1	1:A:16:ARG:NH1	2.33	0.59
1:C:57:PRO:HD3	1:C:170:TYR:HB3	1.84	0.58
1:C:181:LEU:O	1:C:181:LEU:HD12	2.03	0.58
2:D:42:PRO:HG3	5:D:175:HOH:O	2.02	0.58
1:A:246:ASP:HB2	1:A:249:GLU:HG3	1.84	0.58
2:D:76:VAL:O	2:D:78:GLY:N	2.36	0.58
1:C:94:VAL:HG12	1:C:94:VAL:O	2.04	0.58
1:A:226:TRP:CD1	1:A:230:HIS:HD2	2.22	0.57
1:C:78:ASP:HA	5:C:410:HOH:O	2.04	0.57
1:C:152:THR:O	1:C:156:VAL:HG23	2.05	0.57
2:B:57:ARG:NH2	2:B:73:GLU:OE1	2.38	0.57
2:D:45:PHE:CE2	2:D:56:GLY:HA3	2.40	0.57
1:C:134:ASP:HA	2:D:121:LEU:HG	1.87	0.57
1:A:65:ARG:HD3	1:A:65:ARG:C	2.22	0.56
1:A:228:ARG:HG3	1:A:228:ARG:NH1	2.18	0.56
2:B:41:ALA:HB3	2:B:42:PRO:HD3	1.88	0.56
1:A:114:ARG:HB2	1:A:138:TYR:CD1	2.40	0.56
1:C:26:LYS:HZ2	1:C:128:PRO:HD2	1.68	0.56
1:A:129:ILE:O	1:A:132:ARG:HD3	2.06	0.56
2:B:59:ALA:HB2	2:B:73:GLU:CG	2.36	0.56
1:C:266:THR:HA	1:C:269:TYR:O	2.06	0.55
2:B:85:ARG:CZ	2:B:89:GLY:HA2	2.37	0.55
1:C:272:ASP:N	1:C:272:ASP:OD2	2.39	0.55
1:A:101:PRO:O	1:A:118:GLY:HA2	2.05	0.55
1:A:234:ALA:HB3	5:A:403:HOH:O	2.07	0.55
2:D:114:GLU:HG3	2:D:115:LEU:N	2.21	0.55
2:D:76:VAL:C	2:D:78:GLY:H	2.10	0.54
1:A:256:THR:O	1:A:256:THR:HG22	2.08	0.54
2:B:115:LEU:HD22	2:B:118:ALA:O	2.08	0.53
1:A:230:HIS:HB3	1:A:233:SER:HB2	1.91	0.53
2:D:53:ARG:HD2	2:D:55:GLN:OE1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ARG:HB2	1:C:138:TYR:CD1	2.43	0.53
1:A:216:HIS:ND1	5:A:297:HOH:O	2.30	0.53
2:B:52:ARG:HB3	2:B:77:ASP:OD2	2.09	0.52
1:C:17:ARG:HD3	5:C:327:HOH:O	2.08	0.52
2:D:53:ARG:HG3	2:D:53:ARG:O	2.09	0.52
1:A:266:THR:HA	1:A:269:TYR:O	2.09	0.52
2:D:45:PHE:HB3	2:D:105:ARG:NH2	2.25	0.52
2:B:52:ARG:HH22	2:B:119:PRO:HA	1.74	0.52
1:A:159:VAL:HA	1:A:162:ILE:HD12	1.92	0.52
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.73	0.52
1:C:134:ASP:HB2	2:D:119:PRO:O	2.10	0.51
1:A:226:TRP:NE1	1:A:230:HIS:HD2	2.08	0.51
1:C:68:LEU:HD21	1:C:268:TYR:HB3	1.91	0.51
2:D:75:PHE:CE1	2:D:80:GLN:HG3	2.45	0.51
1:C:184:TRP:HZ3	2:D:100:PRO:HG3	1.75	0.51
1:A:155:GLU:O	1:A:158:SER:HB3	2.11	0.51
1:A:203:THR:HG22	2:B:95:VAL:O	2.12	0.50
2:D:67:GLU:HG3	2:D:82:HIS:HD2	1.77	0.50
1:C:58:SER:HB3	1:C:245:VAL:HB	1.92	0.50
1:C:135:SER:HB3	2:D:119:PRO:HD2	1.93	0.50
2:D:81:LEU:HD11	2:D:93:SER:HG	1.76	0.50
1:C:42:ILE:HD11	2:D:97:HIS:CD2	2.47	0.50
1:A:228:ARG:NE	1:A:274:LEU:HD13	2.25	0.50
1:C:242:PRO:O	1:C:243:ASP:HB2	2.12	0.49
1:A:109:ARG:HG3	1:A:111:THR:HG22	1.93	0.49
1:A:65:ARG:HG3	1:A:254:TRP:CE2	2.47	0.49
2:B:101:VAL:HB	2:B:102:PRO:HD2	1.93	0.49
1:C:132:ARG:HG3	1:C:134:ASP:O	2.11	0.49
1:A:111:THR:HG23	1:A:112:ASP:N	2.27	0.49
1:C:100:ALA:HB1	1:C:101:PRO:HD2	1.95	0.49
1:C:140:ARG:O	1:C:199:GLY:HA3	2.13	0.49
1:A:275:GLU:HG2	1:A:276:HIS:H	1.77	0.49
1:C:171:ASN:C	1:C:173:ALA:H	2.16	0.49
1:C:57:PRO:CD	1:C:170:TYR:HB3	2.42	0.48
5:A:369:HOH:O	1:C:30:ARG:HG2	2.13	0.48
1:A:71:GLU:O	1:A:75:GLN:HG3	2.11	0.48
2:B:103:THR:HB	2:B:104:PRO:CD	2.43	0.48
1:C:55:ARG:HH22	2:D:92:ILE:CD1	2.27	0.48
1:A:51:ARG:HD2	1:A:56:SER:HB3	1.95	0.48
2:D:102:PRO:HG2	5:D:170:HOH:O	2.14	0.48
1:A:228:ARG:CG	1:A:228:ARG:HH11	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:VAL:HG23	1:C:208:ASN:HD22	1.79	0.48
1:A:221:LYS:NZ	1:A:273:ALA:O	2.47	0.48
1:A:101:PRO:HG3	1:A:117:ASP:OD2	2.14	0.48
1:A:150:LEU:HD21	1:A:196:TRP:CE3	2.49	0.47
1:A:114:ARG:HB2	1:A:138:TYR:CE1	2.48	0.47
1:A:83:LEU:HD21	1:A:213:TRP:HB3	1.95	0.47
1:A:39:ASN:HA	1:A:42:ILE:HG22	1.97	0.47
1:C:21:ALA:HA	1:C:77:VAL:HG11	1.95	0.47
1:C:6:ASN:HB3	1:C:9:THR:HG23	1.96	0.47
2:D:88:ASP:OD1	2:D:88:ASP:C	2.53	0.47
2:B:57:ARG:HB2	2:B:58:PRO:HD2	1.96	0.46
1:A:64:ARG:NH2	5:A:292:HOH:O	2.32	0.46
2:B:114:GLU:HG3	2:B:115:LEU:N	2.29	0.46
1:A:58:SER:HB3	1:A:245:VAL:HB	1.97	0.46
1:A:206:SER:N	1:A:207:PRO:CD	2.78	0.46
2:D:45:PHE:CD2	2:D:45:PHE:N	2.83	0.46
2:D:52:ARG:HH12	2:D:115:LEU:HB3	1.81	0.46
1:A:65:ARG:HG3	1:A:254:TRP:CZ2	2.51	0.45
2:B:57:ARG:N	2:B:57:ARG:HD3	2.31	0.45
2:D:59:ALA:HA	5:D:155:HOH:O	2.15	0.45
1:C:72:GLN:HE21	1:C:72:GLN:HB2	1.58	0.45
1:A:182:GLU:O	1:A:190:HIS:HB3	2.16	0.45
1:C:13:ASP:OD1	1:C:16:ARG:NH1	2.43	0.45
2:D:42:PRO:HG2	2:D:91:TRP:HZ2	1.82	0.45
1:A:14:GLU:HG2	5:A:461:HOH:O	2.17	0.45
1:C:11:THR:O	1:C:15:LYS:HG3	2.17	0.45
2:D:53:ARG:HD2	2:D:55:GLN:CG	2.47	0.45
1:C:10:LEU:HD13	1:C:14:GLU:HB3	1.99	0.45
1:A:147:VAL:HG12	1:A:196:TRP:HA	1.99	0.45
1:C:166:ASP:OD1	1:C:167:LEU:N	2.47	0.45
2:D:45:PHE:CZ	2:D:105:ARG:HA	2.51	0.45
2:D:43:GLU:HB3	2:D:44:SER:H	1.66	0.45
1:C:121:ALA:HB1	5:C:339:HOH:O	2.15	0.45
1:C:142:SER:OG	1:C:145:GLY:HA3	2.17	0.44
1:A:51:ARG:HD2	1:A:55:ARG:O	2.18	0.44
1:A:168:PRO:HA	1:A:170:TYR:N	2.33	0.44
2:D:91:TRP:O	2:D:100:PRO:HA	2.18	0.44
2:B:105:ARG:CG	2:B:105:ARG:NH2	2.80	0.43
1:C:179:ASN:HB2	5:C:293:HOH:O	2.18	0.43
1:A:232:ASP:N	1:A:232:ASP:OD1	2.51	0.43
1:C:65:ARG:HB2	1:C:262:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ARG:O	1:C:113:GLY:HA2	2.18	0.43
2:D:42:PRO:O	2:D:43:GLU:O	2.37	0.43
2:D:98:TYR:HB2	5:D:136:HOH:O	2.19	0.43
1:C:188:ASN:OD1	1:C:191:ASN:HB2	2.17	0.43
1:C:24:GLU:CD	1:C:27:ARG:HE	2.22	0.43
2:B:81:LEU:HB2	2:B:120:LEU:HD11	2.01	0.43
1:A:133:VAL:HG11	2:B:94:VAL:HG22	2.00	0.43
1:C:51:ARG:HB2	1:C:56:SER:HB3	2.01	0.43
5:A:355:HOH:O	1:C:255:ASN:HB3	2.18	0.43
2:B:59:ALA:HB2	2:B:73:GLU:HG2	2.01	0.43
2:B:97:HIS:O	2:B:97:HIS:CD2	2.72	0.43
2:D:122:PRO:HA	5:D:137:HOH:O	2.19	0.43
1:C:96:ALA:HB3	1:C:98:LEU:HD23	2.00	0.42
1:A:13:ASP:O	1:A:17:ARG:HG3	2.18	0.42
1:C:55:ARG:NH1	2:D:86:ASN:OD1	2.49	0.42
1:C:201:MET:HE2	1:C:211:VAL:HG13	2.01	0.42
1:A:162:ILE:HG21	1:A:176:GLY:C	2.39	0.42
1:C:52:THR:HG23	1:C:245:VAL:CG2	2.50	0.42
2:B:75:PHE:CE2	2:B:80:GLN:HB2	2.54	0.42
2:B:103:THR:HB	2:B:104:PRO:HD2	2.02	0.42
1:C:172:SER:HB2	1:C:184:TRP:CG	2.54	0.42
1:C:171:ASN:O	1:C:173:ALA:N	2.52	0.42
2:B:81:LEU:HB2	2:B:120:LEU:CD1	2.50	0.42
2:D:115:LEU:HD11	2:D:120:LEU:HD21	2.02	0.42
1:A:11:THR:O	1:A:15:LYS:HG3	2.19	0.42
1:A:187:VAL:O	1:A:188:ASN:HB3	2.20	0.42
2:D:114:GLU:O	2:D:116:GLN:HG3	2.20	0.42
1:C:164:ALA:HB1	1:C:167:LEU:HD21	2.01	0.42
2:B:47:GLU:CD	2:B:105:ARG:HE	2.24	0.41
1:C:187:VAL:O	1:C:188:ASN:HB3	2.19	0.41
2:D:67:GLU:HG3	2:D:82:HIS:CD2	2.54	0.41
1:A:94:VAL:CG1	1:A:143:LEU:HD12	2.37	0.41
1:A:111:THR:CG2	1:A:112:ASP:N	2.83	0.41
1:C:97:SER:HB2	5:C:318:HOH:O	2.21	0.41
1:A:25:LEU:CD1	1:A:74:LEU:HD23	2.50	0.41
1:C:26:LYS:HB2	1:C:127:TRP:CZ3	2.55	0.41
1:A:136:ARG:HG2	1:A:138:TYR:CE2	2.56	0.41
1:C:221:LYS:HB2	1:C:271:PHE:CE2	2.55	0.41
2:D:50:LYS:C	2:D:52:ARG:H	2.23	0.41
1:A:193:VAL:O	1:A:197:VAL:HG23	2.20	0.41
1:C:58:SER:C	1:C:61:PRO:HD2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:MET:CE	1:A:211:VAL:HG13	2.50	0.41
1:C:103:PHE:HB3	1:C:104:LEU:H	1.63	0.41
1:A:36:ARG:HB2	1:A:36:ARG:HE	1.71	0.41
1:A:228:ARG:CG	1:A:228:ARG:NH1	2.82	0.41
1:C:134:ASP:CA	2:D:121:LEU:HG	2.51	0.41
1:A:256:THR:HG21	5:A:412:HOH:O	2.20	0.41
1:C:42:ILE:CG2	1:C:43:MET:N	2.84	0.41
1:A:98:LEU:HD11	1:A:211:VAL:HG23	2.02	0.41
1:A:225:GLU:HG2	5:A:358:HOH:O	2.21	0.41
1:A:114:ARG:HG2	1:A:116:MET:SD	2.61	0.41
1:A:182:GLU:O	1:A:191:ASN:OD1	2.40	0.40
1:C:93:THR:C	1:C:95:ARG:H	2.24	0.40
1:C:187:VAL:HG12	5:C:369:HOH:O	2.22	0.40
1:C:174:SER:HA	5:C:295:HOH:O	2.21	0.40
2:B:95:VAL:HG11	2:B:111:ALA:HA	2.02	0.40
2:B:95:VAL:O	2:B:95:VAL:CG1	2.69	0.40
1:A:109:ARG:O	1:A:113:GLY:N	2.51	0.40
1:A:49:GLY:O	1:A:51:ARG:HG2	2.21	0.40
2:B:45:PHE:CE1	2:B:55:GLN:HA	2.57	0.40
1:A:83:LEU:HD21	1:A:213:TRP:CB	2.51	0.40

There are no symmetry-related clashes.

## 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	273/281 (97%)	250 (92%)	20 (7%)	3 (1%)	17	9
1	C	271/281 (96%)	244 (90%)	22 (8%)	5 (2%)	11	4
2	B	67/134 (50%)	64 (96%)	3 (4%)	0	100	100
2	D	71/134 (53%)	59 (83%)	7 (10%)	5 (7%)	1	0
All	All	682/830 (82%)	617 (90%)	52 (8%)	13 (2%)	10	3

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ALA
2	D	43	GLU
2	D	46	ASP
1	C	55	ARG
1	C	172	SER
2	D	77	ASP
2	D	96	SER
1	A	142	SER
1	A	55	ARG
1	C	111	THR
1	C	146	SER
1	C	205	VAL
2	D	51	GLY

### 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	234/240 (98%)	209 (89%)	25 (11%)	8	4
1	C	232/240 (97%)	206 (89%)	26 (11%)	7	3
2	B	56/95 (59%)	51 (91%)	5 (9%)	12	7
2	D	58/95 (61%)	50 (86%)	8 (14%)	4	2
All	All	580/670 (87%)	516 (89%)	64 (11%)	8	4

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	10	LEU
1	A	36	ARG
1	A	40	GLU
1	A	48	SER
1	A	65	ARG
1	A	67	LEU

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Mol	Chain	Res	Type
1	A	76	SER
1	A	83	LEU
1	A	88	TRP
1	A	92	ARG
1	A	95	ARG
1	A	97	SER
1	A	98	LEU
1	A	103	PHE
1	A	110	SER
1	A	132	ARG
1	A	133	VAL
1	A	146	SER
1	A	149	GLU
1	A	158	SER
1	A	163	SER
1	A	215	HIS
1	A	228	ARG
1	A	233	SER
2	B	47	GLU
2	B	55	GLN
2	B	57	ARG
2	B	105	ARG
2	B	114	GLU
1	C	10	LEU
1	C	43	MET
1	C	48	SER
1	C	51	ARG
1	C	52	THR
1	C	83	LEU
1	C	88	TRP
1	C	92	ARG
1	C	97	SER
1	C	98	LEU
1	C	103	PHE
1	C	110	SER
1	C	111	THR
1	C	112	ASP
1	C	114	ARG
1	C	146	SER
1	C	149	GLU
1	C	157	GLU
1	C	174	SER

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Mol	Chain	Res	Type
1	C	185	ARG
1	C	225	GLU
1	C	228	ARG
1	C	252	LYS
1	C	258	ARG
1	C	263	LEU
1	C	272	ASP
2	D	44	SER
2	D	47	GLU
2	D	50	LYS
2	D	53	ARG
2	D	57	ARG
2	D	84	MET
2	D	95	VAL
2	D	114	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	230	HIS
2	B	55	GLN
1	C	54	HIS
1	C	72	GLN
1	C	126	ASN
1	C	180	HIS
1	C	208	ASN
1	C	216	HIS
1	C	248	ASN
1	C	255	ASN
2	D	82	HIS
2	D	97	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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 [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, 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	275/281 (97%)	-0.63	1 (0%) 93 93	5, 14, 28, 68	0
1	C	273/281 (97%)	-0.51	0 100 100	5, 18, 31, 40	0
2	B	71/134 (52%)	-0.12	1 (1%) 78 79	12, 25, 47, 66	0
2	D	75/134 (55%)	0.42	4 (5%) 30 32	17, 38, 54, 66	0
All	All	694/830 (83%)	-0.41	6 (0%) 85 86	5, 19, 41, 68	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	41	ALA	6.9
2	D	68	HIS	4.0
2	D	69	GLY	2.7
1	A	276	HIS	2.6
2	D	67	GLU	2.3
2	D	81	LEU	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
3	NA	C	282	1/1	0.98	0.14	3.90	11,11,11,11	0
3	NA	A	282	1/1	0.99	0.09	1.00	2,2,2,2	0
4	CL	A	283	1/1	0.99	0.06	-1.27	19,19,19,19	0
4	CL	A	284	1/1	0.98	0.05	-2.53	29,29,29,29	0
3	NA	C	283	1/1	0.98	0.04	-4.60	14,14,14,14	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.