



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:42 AM GMT

PDB ID : 2CBT  
Title : CRYSTAL STRUCTURE OF THE NEOCARZINOSTATIN 4TES1 MUTANT BOUND TESTOSTERONE HEMISUCCINATE.  
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Deposited on : 2006-01-06  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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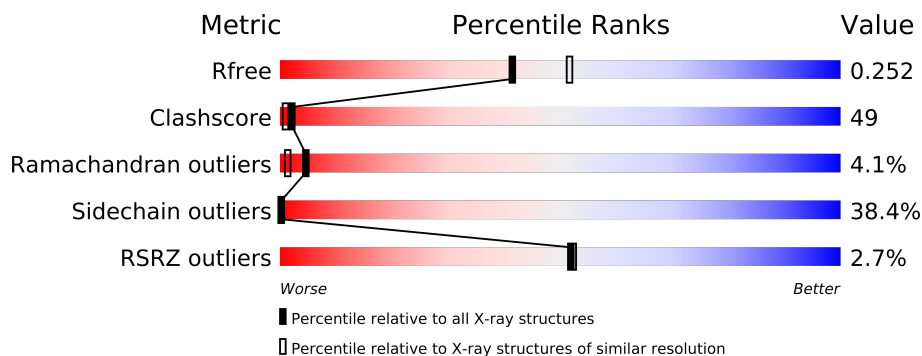
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.20 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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	112	
1	B	112	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	TH2	A	1120	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1664 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

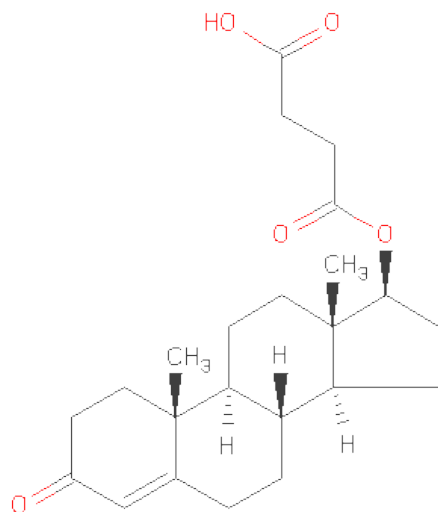
- Molecule 1 is a protein called NEOCARZINOSTATIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	111	Total	C	N	O	S	0	0	0
			789	489	135	163	2			
1	B	111	Total	C	N	O	S	0	0	0
			789	489	135	163	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1033	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
A	1035	ALA	GLY	ENGINEERED MUTATION	UNP P0A3R9
A	1037	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
A	1045	TYR	LEU	ENGINEERED MUTATION	UNP P0A3R9
A	1047	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
A	1052	ILE	PHE	ENGINEERED MUTATION	UNP P0A3R9
A	1078	TRP	PHE	ENGINEERED MUTATION	UNP P0A3R9
A	1094	HIS	GLN	ENGINEERED MUTATION	UNP P0A3R9
A	1096	THR	GLY	ENGINEERED MUTATION	UNP P0A3R9
A	1098	ARG	SER	ENGINEERED MUTATION	UNP P0A3R9
A	1101	LEU	ALA	ENGINEERED MUTATION	UNP P0A3R9
A	1102	SER	GLY	ENGINEERED MUTATION	UNP P0A3R9
B	2033	TRP	ASP	ENGINEERED MUTATION	UNP P0A3R9
B	2035	ALA	GLY	ENGINEERED MUTATION	UNP P0A3R9
B	2037	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
B	2045	TYR	LEU	ENGINEERED MUTATION	UNP P0A3R9
B	2047	SER	CYS	ENGINEERED MUTATION	UNP P0A3R9
B	2052	ILE	PHE	ENGINEERED MUTATION	UNP P0A3R9
B	2078	TRP	PHE	ENGINEERED MUTATION	UNP P0A3R9
B	2094	HIS	GLN	ENGINEERED MUTATION	UNP P0A3R9
B	2096	THR	GLY	ENGINEERED MUTATION	UNP P0A3R9
B	2098	ARG	SER	ENGINEERED MUTATION	UNP P0A3R9
B	2101	LEU	ALA	ENGINEERED MUTATION	UNP P0A3R9
B	2102	SER	GLY	ENGINEERED MUTATION	UNP P0A3R9

- Molecule 2 is TESTOSTERONE HEMISUCCINATE (three-letter code: TH2) (formula:  $C_{23}H_{32}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			28	23	5		
2	B	1	Total	C	O	0	0
			28	23	5		

- Molecule 3 is water.

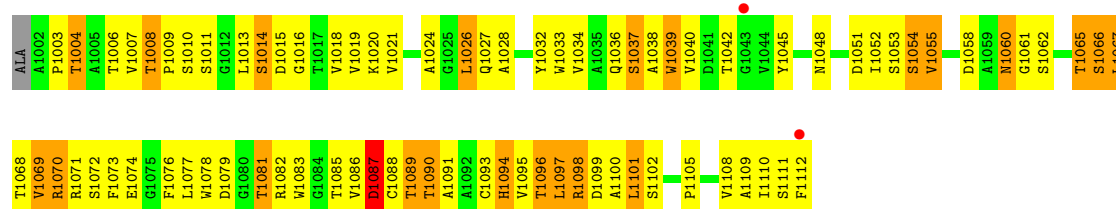
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	14	Total	O	0	0
			14	14		

### 3 Residue-property plots

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.

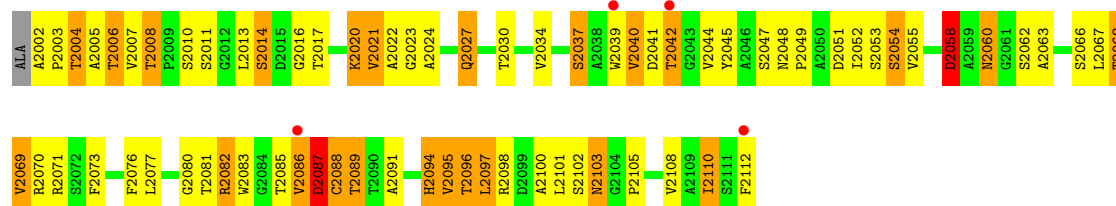
#### • Molecule 1: NEOCARZINOSTATIN

Chain A: 



#### • Molecule 1: NEOCARZINOSTATIN

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.51Å 52.51Å 128.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.20 45.47 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.20) 95.5 (45.47-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 2.20Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.218 , 0.344 0.253 , 0.252	Depositor DCC
$R_{free}$ test set	402 reflections (4.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 70.2	EDS
Estimated twinning fraction	0.469 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 9767 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	1664	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TH2

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	0.30	0/806	0.82	0/1108
1	B	0.34	0/806	0.83	1/1108 (0.1%)
All	All	0.32	0/1612	0.82	1/2216 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2058	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	789	0	748	91	0
1	B	789	0	748	72	0
2	A	28	0	31	3	0
2	B	28	0	31	1	0
3	A	16	0	0	1	0
3	B	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1664	0	1558	155	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 49.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1045:TYR:HH	1:A:1094:HIS:CE1	1.45	1.32
1:A:1045:TYR:OH	1:A:1094:HIS:CE1	1.90	1.22
1:A:1045:TYR:OH	1:A:1094:HIS:NE2	1.73	1.17
1:B:2045:TYR:CE1	1:B:2094:HIS:NE2	2.36	0.93
1:B:2008:THR:HG23	1:B:2020:LYS:HB3	1.50	0.92
1:A:1045:TYR:CZ	1:A:1094:HIS:NE2	2.35	0.86
1:A:1045:TYR:CE1	1:A:1094:HIS:NE2	2.46	0.82
1:B:2017:THR:HB	1:B:2069:VAL:HG23	1.62	0.81
1:B:2045:TYR:HE1	1:B:2094:HIS:NE2	1.81	0.79
1:A:1093:CYS:O	1:A:1110:ILE:HG12	1.83	0.78
1:A:1003:PRO:HA	1:A:1024:ALA:O	1.88	0.74
1:A:1013:LEU:HB2	1:A:1112:PHE:CD2	2.23	0.74
1:B:2004:THR:OG1	1:B:2024:ALA:HB3	1.87	0.73
1:B:2067:LEU:HD12	1:B:2068:THR:H	1.51	0.73
1:A:1076:PHE:HE1	1:B:2054:SER:HB3	1.53	0.73
1:B:2034:VAL:HG12	1:B:2067:LEU:HD22	1.69	0.72
1:A:1094:HIS:HB3	1:A:1109:ALA:HA	1.72	0.69
1:B:2027:GLN:HB3	1:B:2030:THR:OG1	1.93	0.69
1:A:1015:ASP:HA	1:A:1070:ARG:HA	1.74	0.69
1:A:1009:PRO:HD2	1:A:1019:VAL:HG12	1.75	0.69
1:A:1036:GLN:NE2	1:A:1069:VAL:HG12	2.09	0.68
1:B:2094:HIS:HA	1:B:2110:ILE:HG23	1.76	0.68
1:A:1016:GLY:HA2	1:A:1070:ARG:NH1	2.09	0.68
1:A:1009:PRO:O	1:A:1013:LEU:HD21	1.94	0.67
1:A:1077:LEU:HG	1:A:1081:THR:HB	1.77	0.67
1:A:1026:LEU:HG	1:A:1061:GLY:O	1.95	0.67
1:A:1054:SER:HB3	1:B:2076:PHE:HE1	1.58	0.67
1:B:2094:HIS:HB2	1:B:2108:VAL:O	1.95	0.66
1:A:1045:TYR:HE1	1:A:1094:HIS:HE2	1.39	0.66
1:A:1067:LEU:HD12	1:A:1068:THR:H	1.59	0.66
1:A:1018:VAL:HG13	1:A:1067:LEU:O	1.95	0.66
1:A:1101:LEU:HA	2:A:1120:TH2:O24	1.96	0.66
1:B:2067:LEU:HD12	1:B:2068:THR:N	2.12	0.64
1:B:2014:SER:HA	1:B:2071:ARG:NH1	2.12	0.64
1:B:2007:VAL:HG22	1:B:2021:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2017:THR:HB	1:B:2069:VAL:CG2	2.28	0.63
1:A:1034:VAL:HG22	1:A:1097:LEU:CD1	2.29	0.62
1:A:1078:TRP:HH2	1:A:1098:ARG:HD3	1.63	0.62
1:A:1055:VAL:HG23	1:A:1065:THR:HB	1.82	0.61
1:B:2006:THR:HG23	1:B:2022:ALA:HB3	1.83	0.60
1:A:1008:THR:HG23	1:A:1020:LYS:HB3	1.83	0.60
1:B:2016:GLY:HA2	1:B:2070:ARG:NH1	2.17	0.60
1:B:2020:LYS:HE2	1:B:2020:LYS:O	2.01	0.59
1:B:2034:VAL:HB	1:B:2053:SER:HB3	1.83	0.59
1:B:2045:TYR:OH	1:B:2094:HIS:NE2	2.35	0.59
1:A:1008:THR:CG2	1:A:1020:LYS:HE2	2.33	0.59
1:A:1013:LEU:HB2	1:A:1112:PHE:CE2	2.38	0.59
1:A:1026:LEU:O	1:A:1061:GLY:HA3	2.03	0.59
1:A:1110:ILE:HG13	1:A:1112:PHE:CE1	2.39	0.57
1:B:2016:GLY:HA2	1:B:2070:ARG:HH11	1.69	0.57
1:B:2034:VAL:HG22	1:B:2097:LEU:CD1	2.35	0.57
1:A:1004:THR:HG23	1:A:1024:ALA:HB3	1.87	0.57
1:A:1040:VAL:HB	1:A:1083:TRP:CZ2	2.40	0.56
1:B:2077:LEU:HD12	1:B:2081:THR:HB	1.88	0.56
1:A:1014:SER:HA	1:A:1071:ARG:NH1	2.21	0.56
1:A:1094:HIS:HB2	1:A:1108:VAL:O	2.06	0.56
1:A:1007:VAL:HG22	1:A:1021:VAL:HG22	1.87	0.55
1:B:2037:SER:OG	1:B:2096:THR:OG1	2.22	0.55
1:A:1054:SER:HB3	1:B:2076:PHE:CE1	2.41	0.55
1:A:1088:CYS:O	1:A:1089:THR:HG23	2.07	0.55
1:B:2005:ALA:HB2	1:B:2105:PRO:HG2	1.89	0.55
1:B:2045:TYR:HH	1:B:2094:HIS:CE1	2.24	0.55
1:A:1026:LEU:HB3	1:A:1032:TYR:CE1	2.41	0.54
1:A:1004:THR:CG2	1:A:1024:ALA:HB3	2.39	0.53
1:B:2087:ASP:OD1	1:B:2091:ALA:HB3	2.09	0.53
1:A:1072:SER:OG	1:A:1088:CYS:HA	2.08	0.53
1:A:1033:TRP:O	1:A:1097:LEU:HA	2.08	0.53
1:A:1045:TYR:OH	1:A:1094:HIS:HE1	1.79	0.53
2:B:2120:TH2:O20	2:B:2120:TH2:H183	2.08	0.53
1:A:1009:PRO:HG2	1:A:1013:LEU:CD2	2.39	0.52
1:A:1076:PHE:CE1	1:B:2054:SER:HB3	2.39	0.52
1:B:2040:VAL:HG11	1:B:2083:TRP:NE1	2.25	0.52
1:B:2034:VAL:CG1	1:B:2067:LEU:HD22	2.38	0.52
1:A:1073:PHE:CZ	1:A:1086:VAL:HG11	2.45	0.52
1:A:1094:HIS:HA	1:A:1110:ILE:HD13	1.92	0.51
1:A:1100:ALA:O	2:A:1120:TH2:C21	2.58	0.51
1:A:1055:VAL:CG2	1:A:1065:THR:HB	2.40	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1068:THR:HG22	1:A:1068:THR:O	2.10	0.51
1:B:2048:ASN:HB2	1:B:2073:PHE:CD1	2.46	0.51
1:A:1086:VAL:O	1:A:1086:VAL:HG12	2.10	0.50
1:A:1034:VAL:HG22	1:A:1097:LEU:HD11	1.92	0.50
1:B:2017:THR:O	1:B:2069:VAL:HG22	2.12	0.50
1:A:1034:VAL:HG12	1:A:1034:VAL:O	2.11	0.50
1:B:2045:TYR:OH	1:B:2094:HIS:CE1	2.65	0.50
1:B:2101:LEU:O	1:B:2103:ASN:OD1	2.30	0.50
1:A:1037:SER:O	1:A:1093:CYS:HA	2.11	0.50
1:B:2068:THR:O	1:B:2068:THR:HG22	2.12	0.50
1:A:1108:VAL:O	1:A:1108:VAL:HG12	2.11	0.50
1:A:1086:VAL:O	1:A:1087:ASP:O	2.29	0.50
1:A:1078:TRP:CH2	1:A:1098:ARG:HD3	2.45	0.49
1:A:1008:THR:HG21	1:A:1020:LYS:HE2	1.92	0.49
1:A:1037:SER:OG	1:A:1096:THR:OG1	2.30	0.49
1:A:1082:ARG:NH2	1:B:2054:SER:O	2.46	0.49
1:B:2007:VAL:HG21	1:B:2095:VAL:CG2	2.42	0.48
1:A:1079:ASP:HA	1:B:2100:ALA:HB2	1.96	0.48
1:B:2034:VAL:HG22	1:B:2097:LEU:HD11	1.96	0.48
1:A:1100:ALA:O	2:A:1120:TH2:H211	2.13	0.47
1:B:2112:PHE:N	1:B:2112:PHE:CD1	2.82	0.47
1:A:1014:SER:HA	1:A:1071:ARG:CZ	2.43	0.47
1:B:2013:LEU:O	1:B:2112:PHE:HA	2.15	0.47
1:A:1037:SER:HB2	1:A:1045:TYR:CD1	2.50	0.47
1:A:1097:LEU:O	1:A:1105:PRO:HD2	2.14	0.47
1:B:2088:CYS:O	1:B:2089:THR:HG23	2.14	0.47
1:A:1099:ASP:OD2	1:A:1101:LEU:HD12	2.14	0.47
1:A:1016:GLY:HA2	1:A:1070:ARG:HH11	1.79	0.46
1:A:1074:GLU:HG3	3:A:2007:HOH:O	2.15	0.46
1:B:2048:ASN:ND2	1:B:2051:ASP:OD2	2.49	0.46
1:A:1087:ASP:OD1	1:A:1091:ALA:N	2.48	0.46
1:B:2007:VAL:HG21	1:B:2095:VAL:HG21	1.96	0.46
1:B:2023:GLY:O	1:B:2024:ALA:HB2	2.16	0.46
1:A:1054:SER:O	1:B:2082:ARG:NH2	2.49	0.46
1:A:1013:LEU:O	1:A:1071:ARG:NH1	2.49	0.46
1:B:2058:ASP:OD1	1:B:2060:ASN:N	2.50	0.45
1:B:2103:ASN:OD1	1:B:2103:ASN:N	2.50	0.45
1:B:2071:ARG:HE	1:B:2112:PHE:HB3	1.82	0.45
1:A:1052:ILE:HG21	1:B:2049:PRO:HB2	1.98	0.45
1:B:2041:ASP:OD2	1:B:2042:THR:N	2.49	0.45
1:A:1038:ALA:O	1:A:1040:VAL:N	2.50	0.45
1:A:1090:THR:OG1	1:A:1091:ALA:N	2.47	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:2003:PRO:HA	1:B:2024:ALA:O	2.17	0.44
1:A:1028:ALA:HA	1:A:1058:ASP:O	2.17	0.44
1:B:2067:LEU:HD23	1:B:2095:VAL:CG1	2.47	0.44
1:B:2047:SER:O	1:B:2049:PRO:HD3	2.18	0.44
1:A:1065:THR:HG23	1:A:1066:SER:N	2.33	0.44
1:A:1058:ASP:OD1	1:A:1060:ASN:ND2	2.50	0.44
1:B:2087:ASP:OD1	1:B:2091:ALA:N	2.50	0.44
1:A:1079:ASP:OD1	1:A:1081:THR:OG1	2.30	0.44
1:B:2088:CYS:O	1:B:2089:THR:OG1	2.30	0.44
1:A:1098:ARG:HB3	1:A:1098:ARG:HE	1.54	0.44
1:B:2045:TYR:CZ	1:B:2094:HIS:NE2	2.63	0.44
1:A:1024:ALA:O	1:A:1026:LEU:HD23	2.18	0.43
1:A:1053:SER:OG	1:A:1054:SER:N	2.50	0.43
1:A:1013:LEU:HD12	1:A:1112:PHE:CE2	2.53	0.43
1:B:2002:ALA:HB1	1:B:2003:PRO:HD2	2.00	0.43
1:A:1048:ASN:ND2	1:A:1051:ASP:OD2	2.52	0.43
1:B:2008:THR:HG23	1:B:2020:LYS:CB	2.35	0.43
1:A:1033:TRP:N	1:A:1098:ARG:O	2.52	0.43
1:A:1015:ASP:OD1	1:A:1070:ARG:HB3	2.19	0.43
1:B:2101:LEU:HB2	1:B:2103:ASN:OD1	2.18	0.43
1:A:1033:TRP:CH2	1:B:2080:GLY:HA2	2.55	0.42
1:A:1067:LEU:HD12	1:A:1068:THR:N	2.33	0.42
1:B:2020:LYS:HB3	1:B:2020:LYS:HE2	1.51	0.42
1:B:2077:LEU:HD12	1:B:2081:THR:CB	2.49	0.42
1:B:2007:VAL:HG12	1:B:2008:THR:N	2.34	0.42
1:A:1099:ASP:OD1	1:A:1101:LEU:HD12	2.20	0.42
1:B:2049:PRO:HG3	1:B:2076:PHE:CD2	2.55	0.41
1:B:2071:ARG:HE	1:B:2112:PHE:CB	2.33	0.41
1:A:1096:THR:HG22	1:A:1098:ARG:HD2	2.01	0.41
1:B:2108:VAL:HG22	3:B:5014:HOH:O	2.20	0.41
1:B:2041:ASP:HB3	1:B:2044:VAL:HB	2.02	0.41
1:A:1014:SER:HB3	1:A:1071:ARG:HH22	1.85	0.41
1:B:2086:VAL:O	1:B:2087:ASP:O	2.39	0.41
1:B:2004:THR:N	1:B:2024:ALA:O	2.50	0.41
1:A:1007:VAL:HG21	1:A:1095:VAL:HB	2.03	0.41
1:A:1087:ASP:OD1	1:A:1091:ALA:O	2.40	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	109/112 (97%)	89 (82%)	16 (15%)	4 (4%)	5	2
1	B	109/112 (97%)	88 (81%)	16 (15%)	5 (5%)	4	1
All	All	218/224 (97%)	177 (81%)	32 (15%)	9 (4%)	4	1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1039	TRP
1	A	1087	ASP
1	A	1089	THR
1	A	1090	THR
1	B	2058	ASP
1	B	2087	ASP
1	B	2089	THR
1	B	2063	ALA
1	B	2088	CYS

### 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	82/82 (100%)	52 (63%)	30 (37%)	0	0
1	B	82/82 (100%)	49 (60%)	33 (40%)	0	0
All	All	164/164 (100%)	101 (62%)	63 (38%)	0	0

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	THR
1	A	1006	THR
1	A	1008	THR
1	A	1010	SER
1	A	1011	SER
1	A	1014	SER
1	A	1026	LEU
1	A	1027	GLN
1	A	1037	SER
1	A	1039	TRP
1	A	1042	THR
1	A	1054	SER
1	A	1055	VAL
1	A	1060	ASN
1	A	1062	SER
1	A	1065	THR
1	A	1066	SER
1	A	1067	LEU
1	A	1069	VAL
1	A	1070	ARG
1	A	1081	THR
1	A	1085	THR
1	A	1087	ASP
1	A	1094	HIS
1	A	1096	THR
1	A	1097	LEU
1	A	1098	ARG
1	A	1101	LEU
1	A	1102	SER
1	A	1111	SER
1	B	2004	THR
1	B	2006	THR
1	B	2008	THR
1	B	2010	SER
1	B	2011	SER
1	B	2014	SER
1	B	2020	LYS
1	B	2021	VAL
1	B	2027	GLN
1	B	2037	SER
1	B	2039	TRP
1	B	2040	VAL
1	B	2042	THR

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Mol	Chain	Res	Type
1	B	2052	ILE
1	B	2054	SER
1	B	2055	VAL
1	B	2060	ASN
1	B	2062	SER
1	B	2066	SER
1	B	2068	THR
1	B	2069	VAL
1	B	2082	ARG
1	B	2085	THR
1	B	2086	VAL
1	B	2087	ASP
1	B	2094	HIS
1	B	2095	VAL
1	B	2096	THR
1	B	2097	LEU
1	B	2098	ARG
1	B	2102	SER
1	B	2103	ASN
1	B	2110	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1036	GLN
1	B	2060	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

2 ligands are modelled in this entry.

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$
2	TH2	A	1120	-	31,31,31	1.46	6 (19%)	48,48,48	1.94	11 (22%)
2	TH2	B	2120	-	31,31,31	1.56	8 (25%)	48,48,48	1.95	13 (27%)

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
2	TH2	A	1120	-	-	0/9/67/67	0/0/4/4
2	TH2	B	2120	-	-	0/9/67/67	0/0/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2120	TH2	O17-C17	-3.16	1.40	1.46
2	B	2120	TH2	C10-C5	2.92	1.59	1.52
2	A	1120	TH2	C10-C5	2.68	1.59	1.52
2	B	2120	TH2	O17-C20	-2.42	1.26	1.34
2	B	2120	TH2	C8-C9	2.36	1.58	1.53
2	A	1120	TH2	C11-C9	2.33	1.58	1.53
2	B	2120	TH2	C4-C5	2.33	1.37	1.34
2	B	2120	TH2	C11-C9	2.26	1.57	1.53
2	B	2120	TH2	C10-C9	2.14	1.60	1.56
2	A	1120	TH2	C10-C9	2.10	1.60	1.56
2	A	1120	TH2	O3-C3	-2.08	1.19	1.23
2	A	1120	TH2	O17-C17	-2.07	1.42	1.46
2	A	1120	TH2	C8-C9	2.06	1.57	1.53
2	B	2120	TH2	C16-C17	2.02	1.57	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1120	TH2	O17-C17-C16	4.91	123.26	111.03
2	B	2120	TH2	O17-C17-C16	4.87	123.16	111.03
2	A	1120	TH2	C17-O17-C20	4.59	127.94	118.04
2	B	2120	TH2	O17-C17-C13	4.55	122.34	111.20
2	A	1120	TH2	O17-C17-C13	4.52	122.28	111.20
2	A	1120	TH2	C11-C9-C10	-4.24	107.20	113.08
2	B	2120	TH2	C11-C9-C10	-4.13	107.36	113.08
2	B	2120	TH2	C17-O17-C20	3.95	126.57	118.04
2	B	2120	TH2	C12-C11-C9	-3.73	106.91	113.15
2	A	1120	TH2	C12-C11-C9	-3.59	107.14	113.15
2	B	2120	TH2	O17-C20-O20	3.11	131.99	123.65
2	A	1120	TH2	O17-C20-O20	3.05	131.83	123.65
2	A	1120	TH2	C16-C17-C13	-2.83	102.05	105.20
2	B	2120	TH2	C9-C10-C5	-2.56	105.68	109.67
2	A	1120	TH2	C9-C10-C5	-2.41	105.91	109.67
2	B	2120	TH2	C22-C21-C23	-2.41	109.07	113.53
2	A	1120	TH2	O3-C3-C2	2.39	125.18	121.58
2	B	2120	TH2	O3-C3-C2	2.36	125.13	121.58
2	A	1120	TH2	C15-C16-C17	2.29	108.57	104.84
2	A	1120	TH2	O20-C20-C22	-2.27	114.43	123.78
2	B	2120	TH2	O20-C20-C22	-2.26	114.47	123.78
2	B	2120	TH2	C16-C17-C13	-2.20	102.75	105.20
2	B	2120	TH2	C1-C10-C9	2.18	111.50	108.60
2	B	2120	TH2	C15-C16-C17	2.01	108.11	104.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 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	111/112 (99%)	0.17	2 (1%) 65 66	8, 32, 49, 59	0
1	B	111/112 (99%)	0.30	4 (3%) 41 41	13, 33, 54, 83	0
All	All	222/224 (99%)	0.24	6 (2%) 52 52	8, 33, 52, 83	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2039	TRP	5.6
1	A	1112	PHE	4.3
1	B	2042	THR	3.3
1	A	1043	GLY	2.3
1	B	2112	PHE	2.1
1	B	2086	VAL	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TH2	A	1120	28/28	0.19	2.73	5,18,43,62	0
2	TH2	B	2120	28/28	0.17	1.55	3,11,27,37	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.