



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 11:29 pm BST

PDB ID : 2XEC  
Title : Nocardia farcinica maleate cis-trans isomerase bound to TRIS  
Authors : Fisch, F.; Martinez-Fleites, C.; Baudendistel, N.; Hauer, B.; Turkenburg, J.P.;  
Hart, S.; Bruce, N.C.; Grogan, G.  
Deposited on : 2010-05-13  
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

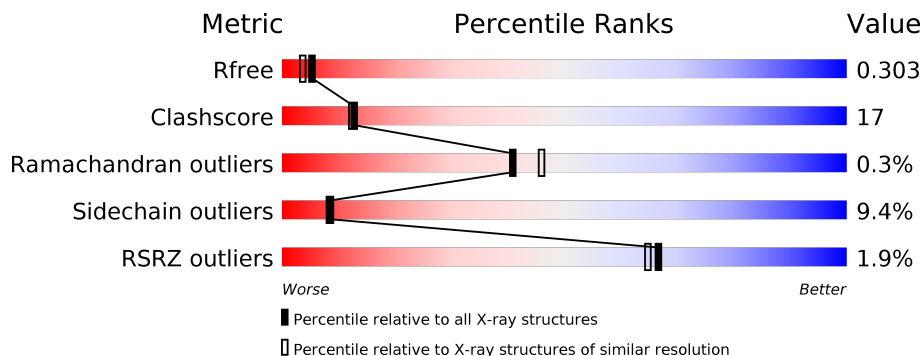
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	273	<p>68% 17% 5% 10%</p>
1	B	273	<p>67% 19% 5% 10%</p>
1	C	273	<p>64% 22% 5% 11%</p>
1	D	273	<p>50% 34% 5% 10%</p>

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
2	TRS	A	300	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 7377 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 PUTATIVE MALEATE ISOMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	246	1818	1136	322	347	13	0	0	0
1	B	245	1812	1132	321	345	14	0	0	0
1	C	243	1800	1125	319	343	13	0	0	0
1	D	245	1810	1130	321	346	13	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q5YXQ1
A	-20	GLY	-	expression tag	UNP Q5YXQ1
A	-19	SER	-	expression tag	UNP Q5YXQ1
A	-18	SER	-	expression tag	UNP Q5YXQ1
A	-17	HIS	-	expression tag	UNP Q5YXQ1
A	-16	HIS	-	expression tag	UNP Q5YXQ1
A	-15	HIS	-	expression tag	UNP Q5YXQ1
A	-14	HIS	-	expression tag	UNP Q5YXQ1
A	-13	HIS	-	expression tag	UNP Q5YXQ1
A	-12	HIS	-	expression tag	UNP Q5YXQ1
A	-11	SER	-	expression tag	UNP Q5YXQ1
A	-10	SER	-	expression tag	UNP Q5YXQ1
A	-9	GLY	-	expression tag	UNP Q5YXQ1
A	-8	LEU	-	expression tag	UNP Q5YXQ1
A	-7	GLU	-	expression tag	UNP Q5YXQ1
A	-6	VAL	-	expression tag	UNP Q5YXQ1
A	-5	LEU	-	expression tag	UNP Q5YXQ1
A	-4	PHE	-	expression tag	UNP Q5YXQ1
A	-3	GLN	-	expression tag	UNP Q5YXQ1
A	-2	GLY	-	expression tag	UNP Q5YXQ1
A	-1	PRO	-	expression tag	UNP Q5YXQ1

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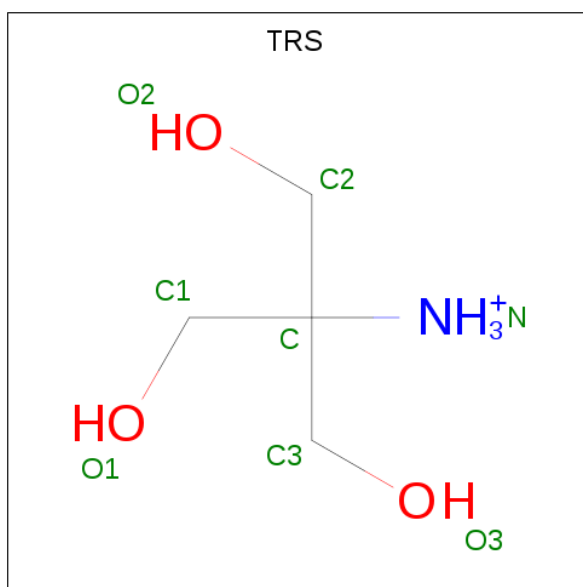
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP Q5YXQ1
B	-21	MET	-	expression tag	UNP Q5YXQ1
B	-20	GLY	-	expression tag	UNP Q5YXQ1
B	-19	SER	-	expression tag	UNP Q5YXQ1
B	-18	SER	-	expression tag	UNP Q5YXQ1
B	-17	HIS	-	expression tag	UNP Q5YXQ1
B	-16	HIS	-	expression tag	UNP Q5YXQ1
B	-15	HIS	-	expression tag	UNP Q5YXQ1
B	-14	HIS	-	expression tag	UNP Q5YXQ1
B	-13	HIS	-	expression tag	UNP Q5YXQ1
B	-12	HIS	-	expression tag	UNP Q5YXQ1
B	-11	SER	-	expression tag	UNP Q5YXQ1
B	-10	SER	-	expression tag	UNP Q5YXQ1
B	-9	GLY	-	expression tag	UNP Q5YXQ1
B	-8	LEU	-	expression tag	UNP Q5YXQ1
B	-7	GLU	-	expression tag	UNP Q5YXQ1
B	-6	VAL	-	expression tag	UNP Q5YXQ1
B	-5	LEU	-	expression tag	UNP Q5YXQ1
B	-4	PHE	-	expression tag	UNP Q5YXQ1
B	-3	GLN	-	expression tag	UNP Q5YXQ1
B	-2	GLY	-	expression tag	UNP Q5YXQ1
B	-1	PRO	-	expression tag	UNP Q5YXQ1
B	0	ALA	-	expression tag	UNP Q5YXQ1
C	-21	MET	-	expression tag	UNP Q5YXQ1
C	-20	GLY	-	expression tag	UNP Q5YXQ1
C	-19	SER	-	expression tag	UNP Q5YXQ1
C	-18	SER	-	expression tag	UNP Q5YXQ1
C	-17	HIS	-	expression tag	UNP Q5YXQ1
C	-16	HIS	-	expression tag	UNP Q5YXQ1
C	-15	HIS	-	expression tag	UNP Q5YXQ1
C	-14	HIS	-	expression tag	UNP Q5YXQ1
C	-13	HIS	-	expression tag	UNP Q5YXQ1
C	-12	HIS	-	expression tag	UNP Q5YXQ1
C	-11	SER	-	expression tag	UNP Q5YXQ1
C	-10	SER	-	expression tag	UNP Q5YXQ1
C	-9	GLY	-	expression tag	UNP Q5YXQ1
C	-8	LEU	-	expression tag	UNP Q5YXQ1
C	-7	GLU	-	expression tag	UNP Q5YXQ1
C	-6	VAL	-	expression tag	UNP Q5YXQ1
C	-5	LEU	-	expression tag	UNP Q5YXQ1
C	-4	PHE	-	expression tag	UNP Q5YXQ1
C	-3	GLN	-	expression tag	UNP Q5YXQ1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q5YXQ1
C	-1	PRO	-	expression tag	UNP Q5YXQ1
C	0	ALA	-	expression tag	UNP Q5YXQ1
D	-21	MET	-	expression tag	UNP Q5YXQ1
D	-20	GLY	-	expression tag	UNP Q5YXQ1
D	-19	SER	-	expression tag	UNP Q5YXQ1
D	-18	SER	-	expression tag	UNP Q5YXQ1
D	-17	HIS	-	expression tag	UNP Q5YXQ1
D	-16	HIS	-	expression tag	UNP Q5YXQ1
D	-15	HIS	-	expression tag	UNP Q5YXQ1
D	-14	HIS	-	expression tag	UNP Q5YXQ1
D	-13	HIS	-	expression tag	UNP Q5YXQ1
D	-12	HIS	-	expression tag	UNP Q5YXQ1
D	-11	SER	-	expression tag	UNP Q5YXQ1
D	-10	SER	-	expression tag	UNP Q5YXQ1
D	-9	GLY	-	expression tag	UNP Q5YXQ1
D	-8	LEU	-	expression tag	UNP Q5YXQ1
D	-7	GLU	-	expression tag	UNP Q5YXQ1
D	-6	VAL	-	expression tag	UNP Q5YXQ1
D	-5	LEU	-	expression tag	UNP Q5YXQ1
D	-4	PHE	-	expression tag	UNP Q5YXQ1
D	-3	GLN	-	expression tag	UNP Q5YXQ1
D	-2	GLY	-	expression tag	UNP Q5YXQ1
D	-1	PRO	-	expression tag	UNP Q5YXQ1
D	0	ALA	-	expression tag	UNP Q5YXQ1

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	8	4	1	3	0	0
2	D	1	8	4	1	3	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	B	1	1	1	0	0
3	D	1	1	1	0	0

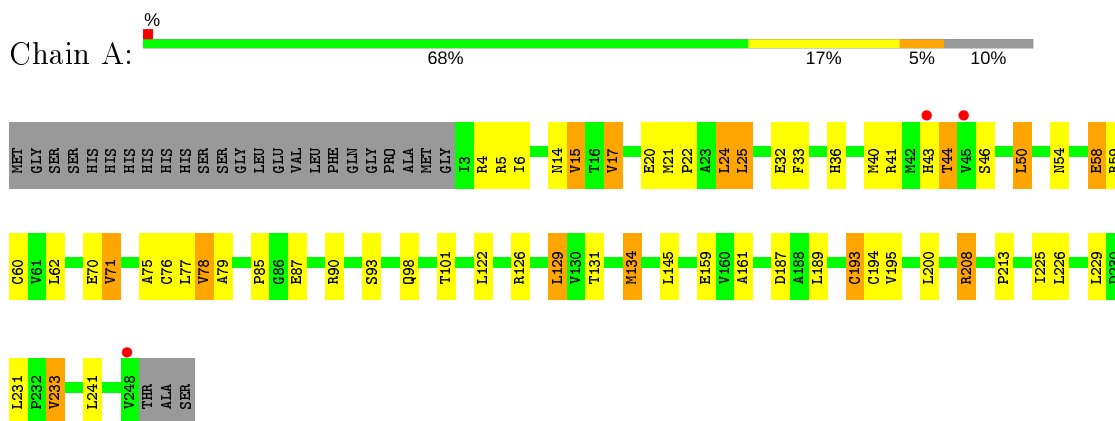
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	49	49	49	0	0
4	B	33	33	33	0	0
4	C	23	23	23	0	0
4	D	14	14	14	0	0

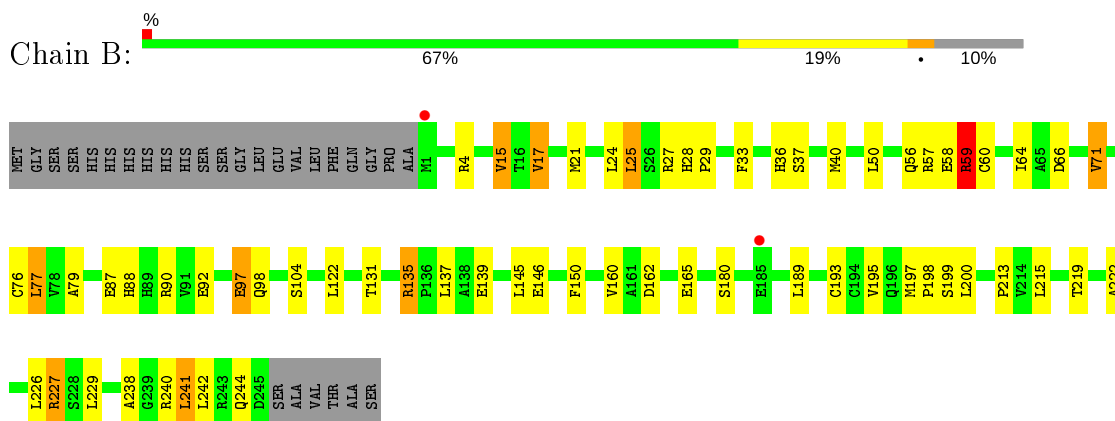
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

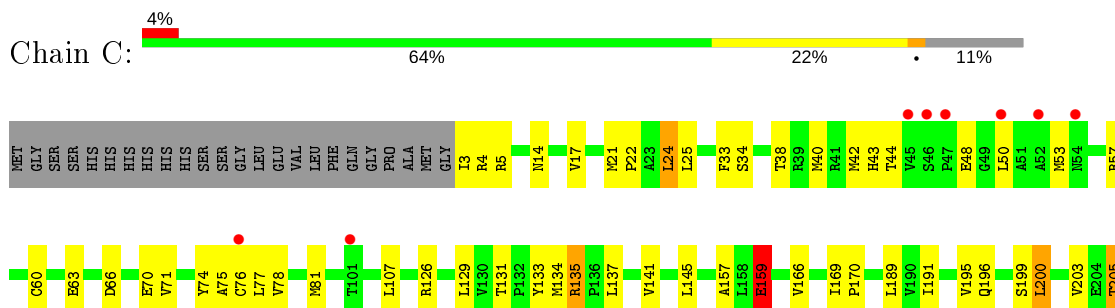
- Molecule 1: PUTATIVE MALEATE ISOMERASE



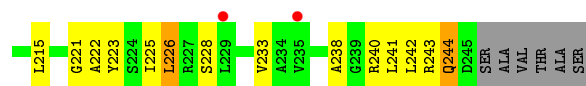
- Molecule 1: PUTATIVE MALEATE ISOMERASE



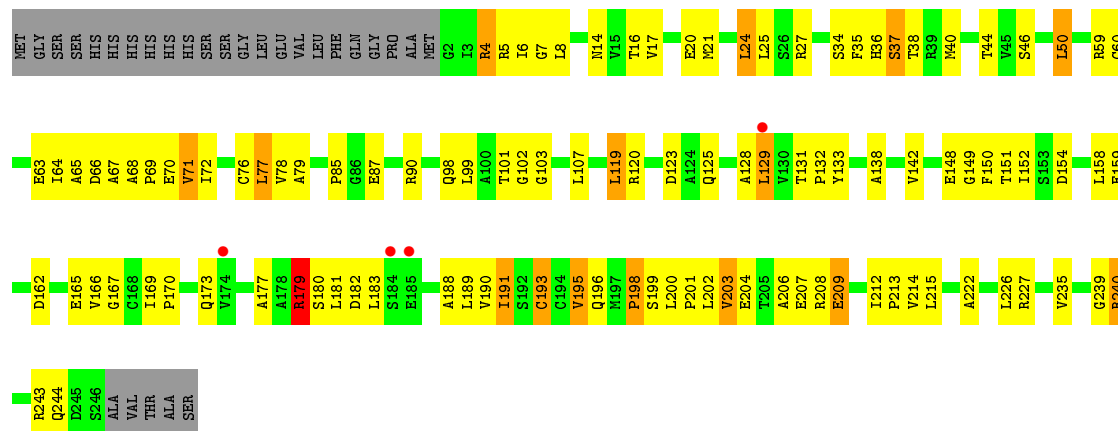
- Molecule 1: PUTATIVE MALEATE ISOMERASE







• Molecule 1: PUTATIVE MALEATE ISOMERASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.16Å 84.51Å 238.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.67 – 2.20 48.67 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.67-2.20) 99.5 (48.67-2.05)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.239 , 0.288 0.254 , 0.303	Depositor DCC
$R_{free}$ test set	2661 reflections (4.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.7	Xtrriage
Anisotropy	0.405	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7377	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.83	0/1846	0.85	4/2514 (0.2%)
1	B	0.79	0/1840	0.83	3/2504 (0.1%)
1	C	0.76	1/1828 (0.1%)	0.81	0/2489
1	D	0.97	5/1838 (0.3%)	0.89	6/2502 (0.2%)
All	All	0.84	6/7352 (0.1%)	0.85	13/10009 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	209	GLU	CD-OE1	19.00	1.46	1.25
1	D	208	ARG	CZ-NH1	9.04	1.44	1.33
1	D	37	SER	CB-OG	-5.23	1.35	1.42
1	D	67	ALA	CA-CB	5.12	1.63	1.52
1	C	159	GLU	CD-OE1	5.11	1.31	1.25
1	D	179	ARG	CD-NE	5.11	1.55	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	71	VAL	CB-CA-C	-7.10	97.91	111.40
1	D	209	GLU	OE1-CD-OE2	6.72	131.36	123.30
1	B	59	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	59	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	D	235	VAL	C-N-CD	-6.09	107.20	120.60
1	D	59	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	59	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	134	MET	CG-SD-CE	5.50	108.99	100.20
1	A	126	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	227	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	D	203	VAL	N-CA-C	5.15	124.91	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	GLY	N-CA-C	5.15	125.97	113.10
1	B	77	LEU	CA-CB-CG	5.12	127.07	115.30

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	1818	0	1843	57	0
1	B	1812	0	1839	45	0
1	C	1800	0	1824	46	0
1	D	1810	0	1832	99	0
2	A	8	0	12	8	0
2	D	8	0	12	4	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	49	0	0	3	0
4	B	33	0	0	6	0
4	C	23	0	0	3	0
4	D	14	0	0	0	0
All	All	7377	0	7362	242	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 17.

All (242) 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:D:98:GLN:O	1:D:101:THR:CG2	1.79	1.28
1:D:98:GLN:O	1:D:101:THR:HG22	1.14	1.28
1:A:98:GLN:O	1:A:101:THR:HG22	1.44	1.17
1:C:42:MET:HB2	1:C:53:MET:HG3	1.42	1.00
1:D:179:ARG:HG3	1:D:179:ARG:HH11	1.28	0.99
1:A:195:VAL:HG23	2:A:300:TR5:H22	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:CG2	2:A:300:TRS:H22	2.00	0.92
1:C:43:HIS:HD2	1:C:44:THR:HG23	1.33	0.90
1:C:71:VAL:HG12	1:C:107:LEU:HB2	1.55	0.89
1:A:40:MET:HE1	1:A:76:CYS:SG	2.15	0.85
1:D:98:GLN:C	1:D:101:THR:HG22	1.96	0.85
1:B:131:THR:HG22	1:B:193:CYS:HB3	1.59	0.84
1:C:221:GLY:O	1:C:225:ILE:HG13	1.81	0.80
1:D:78:VAL:HG12	2:D:300:TRS:N	1.97	0.79
1:A:40:MET:CE	1:A:76:CYS:SG	2.70	0.79
1:B:56:GLN:HE21	1:B:59:ARG:NH1	1.81	0.78
1:D:87:GLU:OE1	1:D:90:ARG:NH2	2.17	0.78
1:D:76:CYS:HB3	1:D:79:ALA:HB3	1.66	0.78
1:D:227:ARG:HH12	1:D:244:GLN:HE21	1.29	0.78
1:D:204:GLU:O	1:D:204:GLU:HG3	1.84	0.76
1:C:43:HIS:CD2	1:C:44:THR:HG23	2.21	0.75
1:A:44:THR:HB	4:A:2011:HOH:O	1.86	0.74
1:C:166:VAL:HG12	1:C:196:GLN:HG3	1.71	0.73
1:C:77:LEU:HA	4:C:2005:HOH:O	1.88	0.73
1:D:166:VAL:O	1:D:169:ILE:HB	1.89	0.73
1:D:207:GLU:OE1	1:D:240:ARG:HD2	1.89	0.72
1:D:177:ALA:O	1:D:180:SER:HB3	1.90	0.70
1:C:78:VAL:CG2	1:C:137:LEU:HD11	2.20	0.70
1:D:240:ARG:H	1:D:240:ARG:HD2	1.55	0.70
1:D:179:ARG:NH1	1:D:179:ARG:HG3	2.05	0.70
1:A:131:THR:HG22	1:A:193:CYS:HB3	1.72	0.69
1:D:196:GLN:O	1:D:198:PRO:HD3	1.92	0.69
1:D:7:GLY:O	1:D:8:LEU:HD23	1.92	0.69
1:C:75:ALA:O	1:C:195:VAL:HG11	1.92	0.69
1:D:14:ASN:HD21	1:D:195:VAL:HG23	1.58	0.68
1:A:129:LEU:HD23	1:A:131:THR:HG23	1.76	0.68
1:A:131:THR:HG22	1:A:193:CYS:CB	2.24	0.67
1:B:87:GLU:OE1	1:B:90:ARG:NH2	2.29	0.66
1:A:4:ARG:NH1	1:A:70:GLU:OE1	2.29	0.65
1:A:85:PRO:O	1:A:90:ARG:NH1	2.30	0.65
1:D:207:GLU:OE2	1:D:239:GLY:HA2	1.97	0.65
1:D:98:GLN:O	1:D:101:THR:HG23	1.89	0.64
1:A:134:MET:HE3	1:A:161:ALA:HB2	1.80	0.63
1:C:134:MET:HA	1:C:159:GLU:HA	1.80	0.63
1:A:134:MET:HE2	1:A:161:ALA:N	2.14	0.63
1:D:21:MET:O	1:D:25:LEU:HB2	1.99	0.63
1:D:5:ARG:HD3	1:D:34:SER:OG	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:GLU:OE1	1:D:243:ARG:NH1	2.22	0.62
1:D:78:VAL:HG12	2:D:300:TRS:HN2	1.64	0.62
1:C:57:ARG:HG3	1:C:74:TYR:HE1	1.64	0.61
1:A:195:VAL:CG2	2:A:300:TRS:C2	2.76	0.61
1:D:14:ASN:ND2	1:D:195:VAL:HG23	2.14	0.61
1:D:40:MET:HG2	1:D:60:CYS:SG	2.41	0.61
1:B:162:ASP:HB3	1:B:165:GLU:HG2	1.83	0.61
1:A:195:VAL:HG22	2:A:300:TRS:C2	2.30	0.60
1:C:42:MET:HG3	1:C:53:MET:HE2	1.83	0.60
1:A:40:MET:HG2	1:A:60:CYS:SG	2.41	0.60
1:C:78:VAL:HG22	1:C:137:LEU:HD11	1.83	0.60
1:B:195:VAL:HA	4:B:2025:HOH:O	2.00	0.60
1:D:131:THR:HG22	1:D:193:CYS:HB2	1.84	0.60
1:B:227:ARG:NH1	1:B:244:GLN:HE21	1.99	0.59
1:D:16:THR:O	1:D:17:VAL:C	2.40	0.59
1:B:222:ALA:O	1:B:226:LEU:HD22	2.03	0.58
1:D:189:LEU:HD23	1:D:190:VAL:N	2.18	0.58
1:D:78:VAL:HG12	2:D:300:TRS:HN3	1.68	0.58
1:B:71:VAL:CG2	1:B:229:LEU:HD21	2.34	0.58
1:A:208:ARG:HH21	1:A:208:ARG:HB3	1.69	0.57
1:D:77:LEU:HG	1:D:193:CYS:O	2.05	0.57
1:B:56:GLN:HE21	1:B:59:ARG:HH11	1.50	0.56
1:C:57:ARG:HG3	1:C:74:TYR:CE1	2.40	0.56
1:A:129:LEU:HD13	1:A:129:LEU:N	2.21	0.56
1:B:58:GLU:HG2	4:B:2008:HOH:O	2.04	0.56
1:B:40:MET:CE	1:B:76:CYS:SG	2.94	0.55
1:C:133:TYR:HB3	1:C:137:LEU:HD23	1.88	0.55
1:C:21:MET:HB3	1:C:22:PRO:HD3	1.88	0.55
1:D:131:THR:HG22	1:D:193:CYS:CB	2.36	0.55
1:B:4:ARG:CZ	4:B:2001:HOH:O	2.55	0.55
1:D:189:LEU:HB3	1:D:214:VAL:HG13	1.89	0.55
1:A:134:MET:CE	1:A:161:ALA:HB2	2.38	0.54
1:A:194:CYS:SG	2:A:300:TRS:H21	2.47	0.54
1:A:78:VAL:H	2:A:300:TRS:H11	1.73	0.54
1:D:129:LEU:HD21	1:D:152:ILE:HG23	1.90	0.54
1:D:64:ILE:O	1:D:65:ALA:C	2.45	0.54
1:C:14:ASN:OD1	1:C:17:VAL:HG13	2.07	0.54
1:C:42:MET:CG	1:C:53:MET:HE2	2.38	0.54
1:A:208:ARG:HB3	1:A:208:ARG:NH2	2.24	0.53
1:A:195:VAL:HG22	2:A:300:TRS:H22	1.81	0.53
1:D:204:GLU:OE2	1:D:243:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ARG:HH11	1:B:244:GLN:NE2	2.07	0.52
1:B:40:MET:HE3	1:B:76:CYS:SG	2.50	0.52
1:D:129:LEU:HD23	1:D:129:LEU:N	2.24	0.52
1:D:24:LEU:O	1:D:27:ARG:HB2	2.10	0.52
1:A:187:ASP:O	1:A:213:PRO:HD2	2.09	0.52
1:A:24:LEU:HD23	1:A:25:LEU:N	2.25	0.52
1:A:87:GLU:HA	1:A:90:ARG:NH2	2.24	0.52
1:A:21:MET:HE3	1:A:225:ILE:HD12	1.92	0.52
1:D:138:ALA:O	1:D:142:VAL:HG23	2.10	0.51
1:C:24:LEU:HD13	1:C:200:LEU:HD21	1.92	0.51
1:B:160:VAL:CG1	1:B:165:GLU:HG3	2.41	0.51
1:D:132:PRO:HA	1:D:158:LEU:HB2	1.91	0.51
1:A:129:LEU:HD23	1:A:131:THR:CG2	2.41	0.50
1:A:21:MET:HB2	1:A:22:PRO:HD3	1.92	0.50
1:D:227:ARG:HH12	1:D:244:GLN:NE2	2.05	0.50
1:A:75:ALA:O	1:A:195:VAL:HG11	2.12	0.50
1:A:41:ARG:HD2	1:B:66:ASP:OD2	2.11	0.50
1:D:240:ARG:H	1:D:240:ARG:CD	2.17	0.50
1:B:25:LEU:HB3	1:B:33:PHE:CD2	2.46	0.50
1:D:38:THR:HG21	1:D:60:CYS:O	2.12	0.50
1:D:189:LEU:O	1:D:215:LEU:HD23	2.13	0.49
1:A:233:VAL:O	1:A:233:VAL:CG2	2.61	0.49
1:A:233:VAL:HG23	1:A:233:VAL:O	2.11	0.49
1:A:54:ASN:ND2	1:A:79:ALA:HB1	2.27	0.49
1:D:239:GLY:O	1:D:243:ARG:HG2	2.13	0.49
1:D:170:PRO:HD2	1:D:173:GLN:HE21	1.78	0.49
1:A:71:VAL:HG22	1:A:229:LEU:HD21	1.95	0.49
1:C:191:ILE:HG22	1:C:215:LEU:O	2.13	0.49
1:D:87:GLU:HA	1:D:90:ARG:NH2	2.27	0.49
1:C:21:MET:O	1:C:25:LEU:HB2	2.13	0.49
1:C:38:THR:CG2	1:C:60:CYS:HB3	2.43	0.49
1:D:182:ASP:C	1:D:182:ASP:OD1	2.51	0.49
1:C:17:VAL:HG12	1:C:195:VAL:O	2.13	0.48
1:A:134:MET:HE1	1:A:159:GLU:O	2.12	0.48
1:B:222:ALA:O	1:B:226:LEU:CD2	2.60	0.48
1:D:65:ALA:O	1:D:68:ALA:N	2.42	0.48
1:B:213:PRO:HD3	1:B:240:ARG:NH2	2.28	0.48
1:D:169:ILE:O	1:D:169:ILE:HG22	2.13	0.48
1:B:219:THR:HB	1:B:242:LEU:CD1	2.44	0.48
1:B:88:HIS:O	1:B:92:GLU:HG3	2.13	0.48
1:C:63:GLU:O	1:C:66:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ARG:NH2	1:D:148:GLU:O	2.40	0.48
1:C:5:ARG:HD3	1:C:34:SER:OG	2.14	0.48
1:A:77:LEU:C	1:A:77:LEU:HD13	2.34	0.48
1:D:69:PRO:HG3	1:D:72:ILE:HG12	1.96	0.48
1:C:135:ARG:HG3	1:C:159:GLU:CD	2.34	0.48
1:D:128:ALA:HB1	1:D:181:LEU:HD13	1.96	0.48
1:D:76:CYS:HA	2:D:300:TRS:H31	1.96	0.48
1:A:54:ASN:OD1	1:A:79:ALA:HB1	2.14	0.47
1:B:135:ARG:O	1:B:139:GLU:HG2	2.15	0.47
1:B:57:ARG:NH1	4:B:2009:HOH:O	2.47	0.47
1:B:71:VAL:HG23	1:B:229:LEU:HD21	1.96	0.47
1:D:71:VAL:HG13	1:D:107:LEU:HB2	1.97	0.47
1:B:17:VAL:HG23	1:B:21:MET:CG	2.44	0.47
1:A:229:LEU:HB2	1:A:231:LEU:CD2	2.44	0.47
1:B:4:ARG:NH2	4:B:2001:HOH:O	2.46	0.47
1:D:119:LEU:HB3	1:D:150:PHE:CZ	2.49	0.47
1:D:14:ASN:OD1	1:D:17:VAL:HG23	2.14	0.47
1:D:191:ILE:HB	1:D:214:VAL:CG1	2.44	0.47
1:D:72:ILE:CD1	1:D:99:LEU:HD21	2.45	0.47
1:A:5:ARG:NH1	4:A:2002:HOH:O	2.40	0.47
1:B:28:HIS:CG	1:B:29:PRO:HD2	2.50	0.47
1:D:214:VAL:HG12	1:D:215:LEU:N	2.30	0.47
1:B:24:LEU:HD11	1:B:238:ALA:CB	2.44	0.47
1:A:77:LEU:HA	4:A:2016:HOH:O	2.15	0.46
1:D:202:LEU:H	1:D:202:LEU:HG	1.50	0.46
1:D:179:ARG:NE	1:D:209:GLU:OE2	2.36	0.46
1:D:200:LEU:HB3	1:D:201:PRO:CD	2.45	0.46
1:D:63:GLU:O	1:D:66:ASP:HB2	2.15	0.46
1:A:129:LEU:HD13	1:A:129:LEU:H	1.80	0.46
1:A:4:ARG:HD2	1:A:70:GLU:OE2	2.15	0.46
1:B:24:LEU:HD13	1:B:200:LEU:HD11	1.98	0.46
1:B:56:GLN:NE2	1:B:59:ARG:NH1	2.59	0.46
1:B:241:LEU:HD13	1:B:242:LEU:HD12	1.98	0.45
1:C:241:LEU:HD13	1:C:241:LEU:C	2.36	0.45
1:D:191:ILE:HG21	1:D:203:VAL:HG22	1.98	0.45
1:C:38:THR:HG21	1:C:60:CYS:HB3	1.97	0.45
1:D:179:ARG:NH1	1:D:179:ARG:CG	2.75	0.45
1:D:46:SER:O	1:D:50:LEU:HB2	2.16	0.45
1:A:14:ASN:OD1	1:A:17:VAL:HG12	2.17	0.45
1:D:162:ASP:HB3	1:D:165:GLU:HG3	1.98	0.45
1:B:227:ARG:NH1	1:B:244:GLN:NE2	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ARG:NH1	1:C:70:GLU:OE1	2.46	0.45
1:D:40:MET:CG	1:D:60:CYS:SG	3.04	0.45
1:A:131:THR:HG22	1:A:193:CYS:HB2	1.95	0.45
1:A:43:HIS:CE1	1:B:66:ASP:OD1	2.70	0.45
1:B:98:GLN:NE2	4:B:2009:HOH:O	2.50	0.45
1:D:206:ALA:CB	1:D:214:VAL:HG21	2.46	0.45
1:D:40:MET:HB2	1:D:40:MET:HE3	1.71	0.44
1:B:57:ARG:HH11	1:B:57:ARG:HG2	1.82	0.44
1:D:85:PRO:O	1:D:90:ARG:NH1	2.50	0.44
1:A:6:ILE:HD11	1:A:33:PHE:HD1	1.82	0.44
1:D:125:GLN:NE2	1:D:149:GLY:O	2.51	0.44
1:A:20:GLU:O	1:A:24:LEU:HD22	2.18	0.44
1:C:131:THR:OG1	1:C:157:ALA:HA	2.17	0.44
1:C:222:ALA:O	1:C:226:LEU:HD22	2.18	0.44
1:C:169:ILE:HA	1:C:170:PRO:HD3	1.81	0.44
1:C:223:TYR:HB2	1:C:241:LEU:HD11	1.98	0.44
1:D:166:VAL:O	1:D:169:ILE:CB	2.63	0.44
1:B:25:LEU:HD12	1:B:25:LEU:HA	1.69	0.44
1:D:129:LEU:CD2	1:D:152:ILE:HG23	2.47	0.44
1:D:21:MET:HE1	1:D:222:ALA:HA	1.99	0.44
1:D:8:LEU:HB2	1:D:37:SER:HB3	1.98	0.44
1:A:46:SER:O	1:A:50:LEU:HD22	2.18	0.43
1:C:25:LEU:HD11	1:C:226:LEU:HD13	2.00	0.43
1:D:170:PRO:HD2	1:D:173:GLN:NE2	2.33	0.43
1:D:182:ASP:OD1	1:D:183:LEU:N	2.51	0.43
1:D:215:LEU:N	1:D:215:LEU:HD23	2.33	0.43
1:D:35:PHE:C	1:D:36:HIS:CG	2.91	0.43
1:A:54:ASN:HD21	1:A:79:ALA:HB1	1.83	0.43
1:A:229:LEU:O	1:A:231:LEU:HD22	2.19	0.43
1:A:15:VAL:HG22	1:B:36:HIS:CE1	2.53	0.43
1:C:33:PHE:CD2	1:C:33:PHE:N	2.86	0.43
1:D:119:LEU:HD12	1:D:119:LEU:HA	1.81	0.43
1:C:240:ARG:HA	1:C:243:ARG:HG3	2.00	0.43
1:C:205:THR:HG23	4:C:2019:HOH:O	2.17	0.43
1:B:197:MET:HA	1:B:198:PRO:HD3	1.76	0.43
1:B:76:CYS:HB3	1:B:79:ALA:HB3	2.01	0.43
1:C:71:VAL:HG11	1:C:228:SER:OG	2.18	0.43
1:A:195:VAL:HG22	2:A:300:TRS:O2	2.18	0.42
1:C:81:MET:SD	1:C:141:VAL:HG13	2.59	0.42
1:C:225:ILE:O	1:C:228:SER:OG	2.23	0.42
1:D:154:ASP:HB3	1:D:181:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ARG:NH1	1:D:244:GLN:HE21	2.07	0.42
1:D:77:LEU:C	1:D:77:LEU:CD1	2.88	0.42
1:B:213:PRO:HD3	1:B:240:ARG:HH21	1.84	0.42
1:B:17:VAL:HG23	1:B:21:MET:HG3	2.01	0.42
1:D:101:THR:HG23	1:D:102:GLY:N	2.35	0.42
1:D:207:GLU:HG2	1:D:212:ILE:O	2.19	0.42
1:D:188:ALA:HA	1:D:213:PRO:O	2.20	0.42
1:C:191:ILE:HG21	1:C:203:VAL:HG22	2.01	0.42
1:D:20:GLU:O	1:D:24:LEU:HD13	2.20	0.42
1:C:238:ALA:HB3	1:C:242:LEU:HD12	2.02	0.41
1:D:17:VAL:HG22	1:D:195:VAL:HG23	2.01	0.41
1:B:146:GLU:HA	1:B:150:PHE:O	2.20	0.41
1:B:97:GLU:CD	1:C:126:ARG:NH1	2.74	0.41
1:C:131:THR:O	1:C:157:ALA:HA	2.20	0.41
1:D:199:SER:O	1:D:202:LEU:HD12	2.19	0.41
1:D:200:LEU:HB3	1:D:201:PRO:HD3	2.02	0.41
1:D:6:ILE:HD13	1:D:6:ILE:N	2.33	0.41
1:A:21:MET:O	1:A:25:LEU:HB2	2.20	0.41
1:C:76:CYS:C	4:C:2005:HOH:O	2.59	0.41
1:D:64:ILE:C	1:D:66:ASP:N	2.71	0.41
1:D:133:TYR:O	1:D:159:GLU:HA	2.21	0.41
1:A:58:GLU:H	1:A:58:GLU:CD	2.24	0.41
1:B:60:CYS:O	1:B:64:ILE:HG22	2.21	0.41
1:D:207:GLU:CD	1:D:240:ARG:HD2	2.41	0.40
1:D:4:ARG:NH1	1:D:70:GLU:OE2	2.55	0.40
1:C:78:VAL:HG21	1:C:137:LEU:HD21	2.02	0.40
1:A:36:HIS:CE1	1:B:15:VAL:HG22	2.56	0.40
1:D:158:LEU:HA	1:D:158:LEU:HD23	1.90	0.40
1:D:204:GLU:O	1:D:204:GLU:CG	2.60	0.40
1:A:129:LEU:O	1:A:129:LEU:HD22	2.21	0.40
1:D:167:GLY:C	1:D:169:ILE:H	2.25	0.40

There are no symmetry-related clashes.

## 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	244/273 (89%)	233 (96%)	11 (4%)	0	100	100
1	B	243/273 (89%)	233 (96%)	9 (4%)	1 (0%)	34	37
1	C	241/273 (88%)	226 (94%)	13 (5%)	2 (1%)	19	19
1	D	243/273 (89%)	225 (93%)	18 (7%)	0	100	100
All	All	971/1092 (89%)	917 (94%)	51 (5%)	3 (0%)	41	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	SER
1	C	199	SER
1	C	244	GLN

### 5.3.2 Protein sidechains [i](#)

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	193/214 (90%)	171 (89%)	22 (11%)	5	5
1	B	192/214 (90%)	173 (90%)	19 (10%)	8	7
1	C	191/214 (89%)	176 (92%)	15 (8%)	12	12
1	D	192/214 (90%)	176 (92%)	16 (8%)	11	11
All	All	768/856 (90%)	696 (91%)	72 (9%)	8	8

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	VAL
1	A	17	VAL
1	A	24	LEU
1	A	25	LEU
1	A	32	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	44	THR
1	A	50	LEU
1	A	58	GLU
1	A	62	LEU
1	A	71	VAL
1	A	78	VAL
1	A	93	SER
1	A	122	LEU
1	A	129	LEU
1	A	145	LEU
1	A	189	LEU
1	A	193	CYS
1	A	200	LEU
1	A	208	ARG
1	A	226	LEU
1	A	233	VAL
1	A	241	LEU
1	B	15	VAL
1	B	17	VAL
1	B	25	LEU
1	B	27	ARG
1	B	37	SER
1	B	50	LEU
1	B	59	ARG
1	B	71	VAL
1	B	77	LEU
1	B	97	GLU
1	B	104	SER
1	B	122	LEU
1	B	135	ARG
1	B	137	LEU
1	B	145	LEU
1	B	180	SER
1	B	189	LEU
1	B	215	LEU
1	B	241	LEU
1	C	3	ILE
1	C	24	LEU
1	C	40	MET
1	C	48	GLU
1	C	50	LEU
1	C	129	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	135	ARG
1	C	145	LEU
1	C	159	GLU
1	C	189	LEU
1	C	200	LEU
1	C	205	THR
1	C	226	LEU
1	C	233	VAL
1	C	244	GLN
1	D	4	ARG
1	D	24	LEU
1	D	44	THR
1	D	50	LEU
1	D	77	LEU
1	D	119	LEU
1	D	123	ASP
1	D	129	LEU
1	D	151	THR
1	D	179	ARG
1	D	191	ILE
1	D	193	CYS
1	D	195	VAL
1	D	198	PRO
1	D	226	LEU
1	D	240	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	98	GLN
1	A	244	GLN
1	B	56	GLN
1	B	98	GLN
1	B	125	GLN
1	B	244	GLN
1	C	43	HIS
1	C	125	GLN
1	C	244	GLN
1	D	173	GLN
1	D	244	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z  > 2$
2	TRS	D	300	-	7,7,7	0.53	0	9,9,9	0.99	0
2	TRS	A	300	-	7,7,7	0.78	0	9,9,9	1.63	1 (11%)

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	TRS	D	300	-	-	9/9/9/9	-
2	TRS	A	300	-	-	5/9/9/9	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	300	TRS	O3-C3-C	3.52	122.15	111.00

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	300	TRS	C2-C-C1-O1
2	D	300	TRS	C1-C-C2-O2
2	D	300	TRS	C3-C-C2-O2
2	D	300	TRS	C2-C-C3-O3
2	D	300	TRS	C1-C-C3-O3
2	A	300	TRS	C1-C-C2-O2
2	D	300	TRS	C3-C-C1-O1
2	D	300	TRS	N-C-C2-O2
2	D	300	TRS	N-C-C3-O3
2	A	300	TRS	N-C-C3-O3
2	A	300	TRS	C1-C-C3-O3
2	A	300	TRS	C2-C-C3-O3
2	D	300	TRS	N-C-C1-O1
2	A	300	TRS	N-C-C2-O2

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	300	TRS	4	0
2	A	300	TRS	8	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	246/273 (90%)	-0.12	3 (1%) 79 77	28, 41, 61, 80	0
1	B	245/273 (89%)	-0.20	2 (0%) 86 85	29, 45, 62, 73	0
1	C	243/273 (89%)	0.09	10 (4%) 37 35	30, 54, 91, 114	0
1	D	245/273 (89%)	0.19	4 (1%) 72 70	31, 66, 114, 142	0
All	All	979/1092 (89%)	-0.01	19 (1%) 66 65	28, 49, 96, 142	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	46	SER	10.0
1	C	45	VAL	7.6
1	C	47	PRO	6.1
1	B	1	MET	4.5
1	D	185	GLU	4.3
1	D	184	SER	4.1
1	B	185	GLU	3.3
1	A	248	VAL	3.2
1	A	45	VAL	3.0
1	C	235	VAL	2.9
1	C	52	ALA	2.9
1	D	174	VAL	2.7
1	C	76	CYS	2.6
1	C	54	ASN	2.6
1	C	101	THR	2.5
1	C	229	LEU	2.5
1	C	50	LEU	2.3
1	D	129	LEU	2.2
1	A	43	HIS	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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	TRS	A	300	8/8	0.64	0.26	42,44,46,46	0
2	TRS	D	300	8/8	0.76	0.26	41,45,47,47	0
3	CA	D	1247	1/1	0.93	0.13	54,54,54,54	0
3	CA	B	1246	1/1	0.96	0.04	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.