



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:03 AM GMT

PDB ID : 4DK1  
Title : Crystal Structure of MacA-MexA chimeric protein, containing the Pseudomonas aeruginosa MexA alpha-hairpin domain.  
Authors : Xu, Y.; Ha, N.C.  
Deposited on : 2012-02-03  
Resolution : 3.50 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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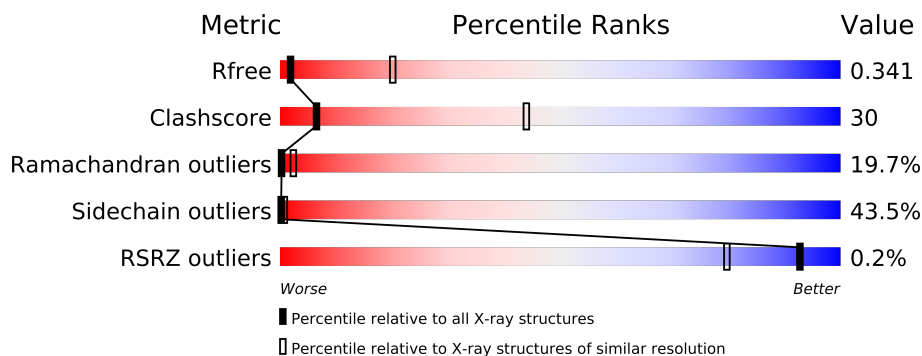
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.50 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	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)

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	341	
1	B	341	
1	C	341	
1	D	341	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8568 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 Putative MacA, Multidrug resistance protein mexA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	Se	4	0	0
			2108	1316	355	435	2			
1	B	285	Total	C	N	O	Se	4	0	0
			2191	1369	369	451	2			
1	C	278	Total	C	N	O	Se	4	0	0
			2135	1336	358	439	2			
1	D	278	Total	C	N	O	Se	4	0	0
			2134	1334	359	439	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	EXPRESSION TAG	UNP Q2EHL9
A	27	ALA	-	EXPRESSION TAG	UNP Q2EHL9
A	28	MSE	-	EXPRESSION TAG	UNP Q2EHL9
A	29	ASP	-	EXPRESSION TAG	UNP Q2EHL9
A	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
A	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
B	26	GLY	-	EXPRESSION TAG	UNP Q2EHL9
B	27	ALA	-	EXPRESSION TAG	UNP Q2EHL9
B	28	MSE	-	EXPRESSION TAG	UNP Q2EHL9
B	29	ASP	-	EXPRESSION TAG	UNP Q2EHL9
B	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
B	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
C	26	GLY	-	EXPRESSION TAG	UNP Q2EHL9
C	27	ALA	-	EXPRESSION TAG	UNP Q2EHL9
C	28	MSE	-	EXPRESSION TAG	UNP Q2EHL9
C	29	ASP	-	EXPRESSION TAG	UNP Q2EHL9
C	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
C	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9
D	26	GLY	-	EXPRESSION TAG	UNP Q2EHL9
D	27	ALA	-	EXPRESSION TAG	UNP Q2EHL9
D	28	MSE	-	EXPRESSION TAG	UNP Q2EHL9

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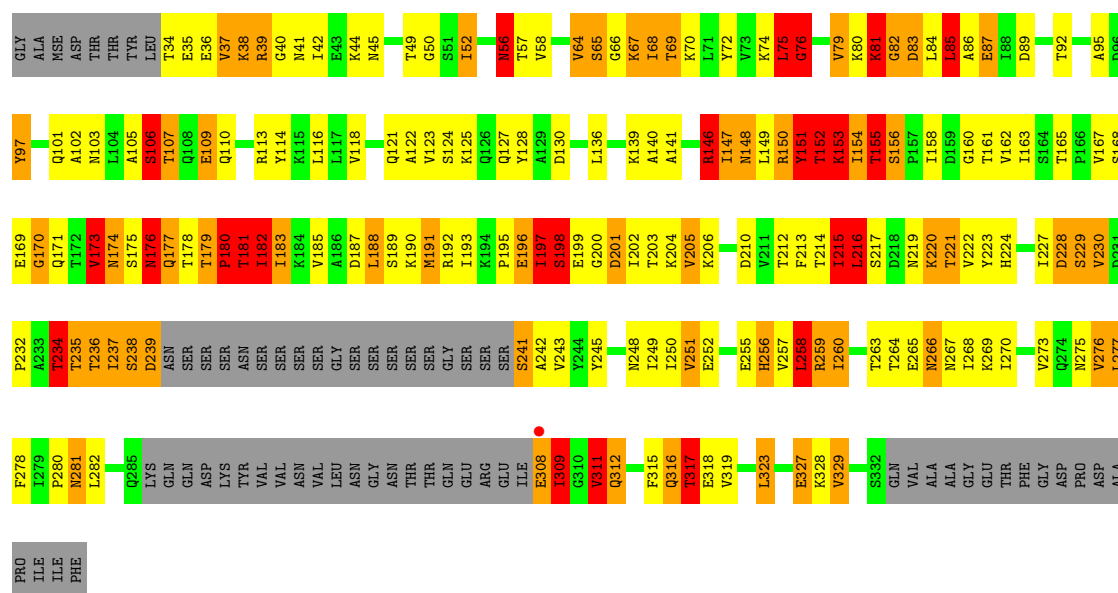
Chain	Residue	Modelled	Actual	Comment	Reference
D	29	ASP	-	EXPRESSION TAG	UNP Q2EHL9
D	68	ILE	VAL	SEE REMARK 999	UNP Q2EHL9
D	85	LEU	ILE	SEE REMARK 999	UNP Q2EHL9

### 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.

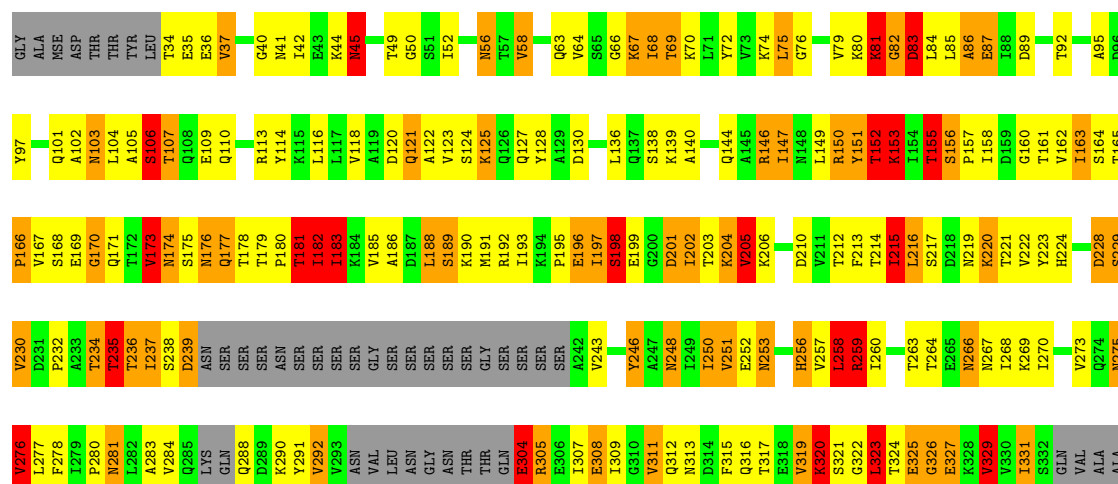
- Molecule 1: Putative MacA, Multidrug resistance protein mexA

Chain A:



- Molecule 1: Putative MacA, Multidrug resistance protein mexA

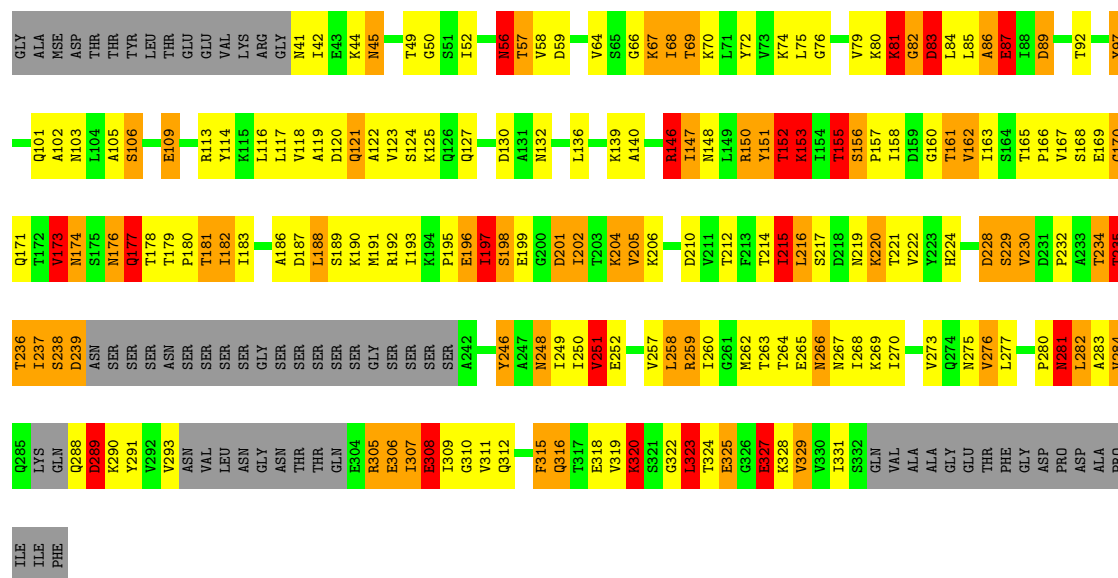
Chain B:



GLY  
GLU  
THR  
PHE  
GLY  
ASP  
PRO  
ASP  
ALA  
PRO  
ILE  
ILE  
PHE

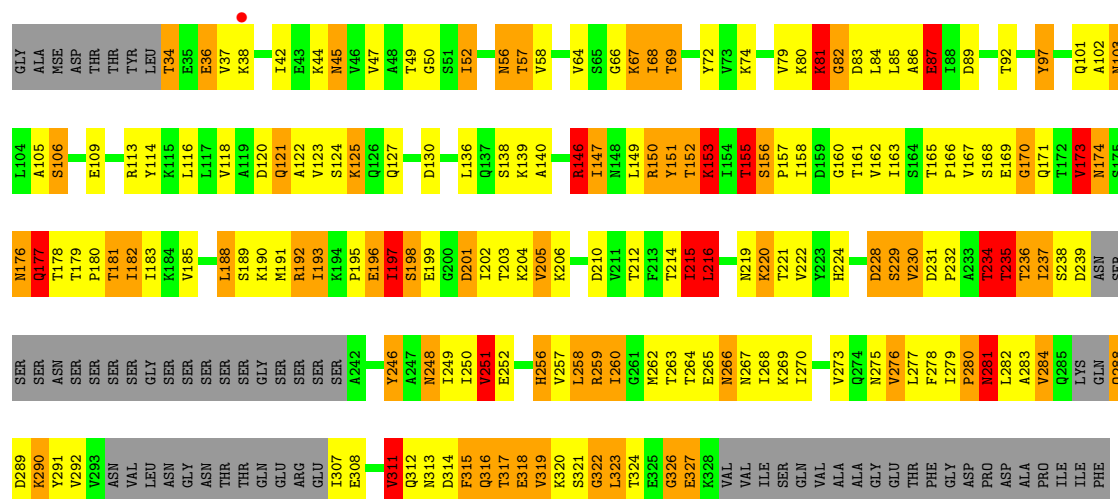
• Molecule 1: Putative MacA, Multidrug resistance protein mexA

Chain C:



• Molecule 1: Putative MacA, Multidrug resistance protein mexA

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.71Å 151.71Å 216.95Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.95 – 3.50 19.95 – 3.50	Depositor EDS
% Data completeness (in resolution range)	91.3 (19.95-3.50) 91.4 (19.95-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.80 (at 3.52Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.314 , 0.368 0.289 , 0.341	Depositor DCC
$R_{free}$ test set	1706 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.4	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.13 , -20.0	EDS
Estimated twinning fraction	0.279 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.30$ , $\langle L^2 \rangle = 0.14$	Xtriage
Outliers	4 of 33690 reflections (0.012%)	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	8568	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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 ⓘ

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	1.23	11/2127 (0.5%)	1.47	15/2884 (0.5%)
1	B	1.22	7/2210 (0.3%)	1.44	20/2994 (0.7%)
1	C	0.97	1/2154 (0.0%)	1.35	13/2920 (0.4%)
1	D	1.00	2/2153 (0.1%)	1.35	14/2917 (0.5%)
All	All	1.11	21/8644 (0.2%)	1.41	62/11715 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	23
1	B	0	25
1	C	0	22
1	D	0	24
All	All	0	94

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	196	GLU	CG-CD	9.57	1.66	1.51
1	A	196	GLU	CG-CD	8.69	1.65	1.51
1	B	45	ASN	CG-ND2	-6.84	1.15	1.32
1	A	196	GLU	CB-CG	6.58	1.64	1.52
1	B	121	GLN	CD-NE2	-6.55	1.16	1.32
1	A	316	GLN	CG-CD	6.50	1.66	1.51
1	B	58	VAL	CA-CB	-6.23	1.41	1.54
1	D	196	GLU	CG-CD	6.17	1.61	1.51
1	A	151	TYR	CE2-CZ	6.13	1.46	1.38
1	B	253	ASN	CG-ND2	5.97	1.47	1.32
1	A	179	THR	C-O	-5.95	1.12	1.23
1	A	308	GLU	CB-CG	5.61	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	308	GLU	CG-CD	5.61	1.60	1.51
1	A	245	TYR	CB-CG	-5.59	1.43	1.51
1	B	121	GLN	CD-OE1	-5.58	1.11	1.24
1	A	79	VAL	CB-CG2	5.56	1.64	1.52
1	A	173	VAL	CB-CG1	-5.43	1.41	1.52
1	C	196	GLU	CG-CD	5.38	1.60	1.51
1	A	154	ILE	CB-CG2	-5.14	1.36	1.52
1	D	196	GLU	CB-CG	5.11	1.61	1.52
1	B	186	ALA	CA-CB	-5.05	1.41	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	ARG	NE-CZ-NH2	16.43	128.51	120.30
1	C	146	ARG	NE-CZ-NH1	16.19	128.40	120.30
1	D	146	ARG	NE-CZ-NH1	16.14	128.37	120.30
1	B	146	ARG	NE-CZ-NH2	14.79	127.70	120.30
1	D	146	ARG	NE-CZ-NH2	-14.74	112.93	120.30
1	C	146	ARG	NE-CZ-NH2	-14.59	113.00	120.30
1	A	146	ARG	NE-CZ-NH1	-13.13	113.73	120.30
1	B	146	ARG	NE-CZ-NH1	-11.50	114.55	120.30
1	B	189	SER	N-CA-C	-9.29	85.91	111.00
1	B	323	LEU	CB-CG-CD1	-9.23	95.31	111.00
1	C	189	SER	N-CA-C	-8.88	87.03	111.00
1	A	189	SER	N-CA-C	-8.79	87.25	111.00
1	D	189	SER	N-CA-C	-8.29	88.61	111.00
1	A	323	LEU	N-CA-C	-7.64	90.36	111.00
1	A	76	GLY	N-CA-C	-7.05	95.47	113.10
1	D	146	ARG	CD-NE-CZ	6.79	133.10	123.60
1	D	177	GLN	CA-CB-CG	6.65	128.02	113.40
1	A	177	GLN	CA-CB-CG	6.62	127.97	113.40
1	A	216	LEU	CA-CB-CG	6.51	130.28	115.30
1	C	289	ASP	N-CA-C	6.48	128.49	111.00
1	B	323	LEU	N-CA-C	6.44	128.39	111.00
1	B	177	GLN	CA-CB-CG	6.43	127.55	113.40
1	C	177	GLN	CA-CB-CG	6.43	127.54	113.40
1	B	320	LYS	N-CA-C	-6.39	93.75	111.00
1	D	322	GLY	N-CA-C	-6.33	97.26	113.10
1	A	146	ARG	CD-NE-CZ	6.32	132.45	123.60
1	A	243	VAL	CB-CA-C	-6.29	99.44	111.40
1	A	309	ILE	N-CA-C	6.29	127.99	111.00
1	D	216	LEU	CA-CB-CG	6.18	129.51	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	VAL	CB-CA-C	-6.17	99.69	111.40
1	D	57	THR	CB-CA-C	-6.15	94.99	111.60
1	C	323	LEU	N-CA-C	6.11	127.48	111.00
1	D	323	LEU	N-CA-C	6.02	127.25	111.00
1	C	146	ARG	CD-NE-CZ	5.97	131.96	123.60
1	B	323	LEU	CA-CB-CG	-5.82	101.91	115.30
1	D	192	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	193	ILE	CG1-CB-CG2	-5.76	98.73	111.40
1	B	146	ARG	CD-NE-CZ	5.75	131.66	123.60
1	B	215	ILE	CB-CA-C	-5.75	100.10	111.60
1	B	258	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	B	259	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	B	75	LEU	CB-CG-CD1	5.65	120.61	111.00
1	D	313	ASN	N-CA-C	5.65	126.25	111.00
1	C	162	VAL	CB-CA-C	-5.60	100.75	111.40
1	B	83	ASP	N-CA-C	5.56	126.00	111.00
1	D	177	GLN	CB-CA-C	5.53	121.46	110.40
1	D	162	VAL	CB-CA-C	-5.45	101.05	111.40
1	C	177	GLN	CB-CA-C	5.44	121.28	110.40
1	A	311	VAL	N-CA-C	5.43	125.66	111.00
1	C	312	GLN	N-CA-C	5.43	125.65	111.00
1	B	243	VAL	CB-CA-C	-5.41	101.12	111.40
1	C	89	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	198	SER	N-CA-C	5.35	125.45	111.00
1	B	75	LEU	CB-CG-CD2	-5.34	101.92	111.00
1	A	243	VAL	N-CA-C	5.34	125.43	111.00
1	A	198	SER	N-CA-C	5.34	125.41	111.00
1	B	179	THR	CB-CA-C	-5.27	97.38	111.60
1	A	65	SER	N-CA-C	-5.25	96.83	111.00
1	D	215	ILE	CB-CA-C	-5.21	101.17	111.60
1	C	83	ASP	N-CA-C	5.14	124.87	111.00
1	B	183	ILE	CG1-CB-CG2	-5.05	100.30	111.40
1	C	57	THR	CB-CA-C	-5.03	98.03	111.60

There are no chirality outliers.

All (94) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	VAL	Peptide
1	A	153	LYS	Peptide
1	A	180	PRO	Peptide
1	A	181	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	188	LEU	Peptide
1	A	215	ILE	Peptide
1	A	230	VAL	Peptide
1	A	238	SER	Peptide
1	A	241	SER	Peptide
1	A	259	ARG	Peptide
1	A	280	PRO	Peptide
1	A	281	ASN	Peptide
1	A	308	GLU	Peptide
1	A	311	VAL	Peptide
1	A	312	GLN	Peptide
1	A	317	THR	Peptide
1	A	323	LEU	Peptide
1	A	37	VAL	Peptide
1	A	39	ARG	Peptide
1	A	56	ASN	Peptide
1	A	75	LEU	Peptide
1	A	85	LEU	Mainchain,Peptide
1	B	120	ASP	Peptide
1	B	123	VAL	Peptide
1	B	153	LYS	Peptide
1	B	166	PRO	Peptide
1	B	181	THR	Peptide
1	B	188	LEU	Peptide
1	B	230	VAL	Peptide
1	B	250	ILE	Peptide
1	B	256	HIS	Peptide
1	B	259	ARG	Peptide
1	B	280	PRO	Peptide
1	B	281	ASN	Peptide
1	B	283	ALA	Peptide
1	B	284	VAL	Peptide
1	B	290	LYS	Peptide
1	B	292	VAL	Peptide
1	B	304	GLU	Peptide
1	B	307	ILE	Peptide
1	B	308	GLU	Peptide
1	B	311	VAL	Peptide
1	B	319	VAL	Peptide
1	B	322	GLY	Peptide
1	B	329	VAL	Peptide
1	B	45	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	56	ASN	Peptide
1	C	120	ASP	Peptide
1	C	123	VAL	Peptide
1	C	153	LYS	Peptide
1	C	166	PRO	Peptide
1	C	181	THR	Peptide
1	C	188	LEU	Peptide
1	C	215	ILE	Peptide
1	C	230	VAL	Peptide
1	C	259	ARG	Peptide
1	C	280	PRO	Peptide
1	C	281	ASN	Peptide
1	C	282	LEU	Peptide
1	C	288	GLN	Peptide
1	C	306	GLU	Peptide
1	C	308	GLU	Peptide
1	C	311	VAL	Peptide
1	C	319	VAL	Peptide
1	C	320	LYS	Peptide
1	C	322	GLY	Peptide
1	C	45	ASN	Peptide
1	C	56	ASN	Peptide
1	C	87	GLU	Peptide
1	D	120	ASP	Peptide
1	D	123	VAL	Peptide
1	D	153	LYS	Peptide
1	D	166	PRO	Peptide
1	D	181	THR	Peptide
1	D	188	LEU	Peptide
1	D	230	VAL	Peptide
1	D	256	HIS	Peptide
1	D	259	ARG	Peptide
1	D	280	PRO	Peptide
1	D	281	ASN	Peptide
1	D	288	GLN	Peptide
1	D	291	TYR	Peptide
1	D	308	GLU	Peptide
1	D	311	VAL	Peptide
1	D	318	GLU	Peptide
1	D	319	VAL	Peptide
1	D	322	GLY	Peptide
1	D	323	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	D	326	GLY	Peptide
1	D	45	ASN	Peptide
1	D	47	VAL	Peptide
1	D	56	ASN	Peptide
1	D	87	GLU	Peptide

## 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	2108	0	0	69	2
1	B	2191	0	0	69	2
1	C	2135	0	0	63	1
1	D	2134	0	0	62	1
All	All	8568	0	0	255	3

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 30.

All (255) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:67:LYS:NZ	1:C:68:ILE:O	1.89	1.05
1:A:67:LYS:NZ	1:A:68:ILE:O	1.89	1.05
1:D:67:LYS:NZ	1:D:68:ILE:O	1.89	1.05
1:A:195:PRO:O	1:A:197:ILE:N	1.97	0.97
1:B:67:LYS:NZ	1:B:68:ILE:O	1.99	0.95
1:A:201:ASP:N	1:A:201:ASP:OD2	1.94	0.95
1:B:201:ASP:OD2	1:B:201:ASP:N	2.00	0.93
1:B:168:SER:N	1:B:171:GLN:OE1	2.01	0.93
1:B:40:GLY:N	1:B:276:VAL:O	2.00	0.92
1:C:174:ASN:ND2	1:D:176:ASN:O	2.03	0.92
1:B:198:SER:OG	1:B:199:GLU:N	1.93	0.91
1:A:174:ASN:ND2	1:B:176:ASN:O	2.04	0.91
1:A:198:SER:OG	1:A:199:GLU:N	2.02	0.86
1:C:201:ASP:N	1:C:201:ASP:OD2	2.08	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:201:ASP:N	1:D:201:ASP:OD2	2.10	0.85
1:B:151:TYR:O	1:B:153:LYS:N	2.11	0.83
1:A:168:SER:N	1:A:171:GLN:OE1	2.12	0.83
1:B:156:SER:OG	1:B:156:SER:O	1.94	0.82
1:D:316:GLN:N	1:D:316:GLN:OE1	2.14	0.81
1:C:151:TYR:O	1:C:153:LYS:N	2.13	0.81
1:B:178:THR:O	1:B:178:THR:OG1	1.94	0.80
1:D:281:ASN:O	1:D:283:ALA:N	2.15	0.80
1:D:195:PRO:O	1:D:197:ILE:N	2.15	0.78
1:B:195:PRO:O	1:B:197:ILE:N	2.16	0.78
1:C:195:PRO:O	1:C:197:ILE:N	2.16	0.78
1:D:234:THR:O	1:D:236:THR:N	2.17	0.77
1:D:168:SER:N	1:D:171:GLN:OE1	2.16	0.77
1:D:198:SER:OG	1:D:199:GLU:N	2.14	0.77
1:A:277:LEU:O	1:A:319:VAL:N	2.17	0.77
1:C:234:THR:O	1:C:234:THR:OG1	2.01	0.76
1:C:198:SER:OG	1:C:199:GLU:N	2.17	0.76
1:C:168:SER:N	1:C:171:GLN:OE1	2.20	0.75
1:A:234:THR:OG1	1:A:234:THR:O	2.01	0.75
1:C:178:THR:OG1	1:C:178:THR:O	2.00	0.75
1:D:165:THR:OG1	1:D:165:THR:O	1.99	0.74
1:B:264:THR:OG1	1:B:266:ASN:ND2	2.21	0.74
1:D:151:TYR:O	1:D:153:LYS:N	2.21	0.73
1:A:151:TYR:O	1:A:153:LYS:N	2.21	0.73
1:D:156:SER:O	1:D:156:SER:OG	2.02	0.73
1:D:281:ASN:OD1	1:D:315:PHE:CG	2.42	0.73
1:C:316:GLN:OE1	1:C:316:GLN:N	2.24	0.71
1:A:311:VAL:N	1:A:318:GLU:OE2	2.23	0.71
1:C:217:SER:OG	1:D:199:GLU:O	2.08	0.70
1:C:234:THR:O	1:C:236:THR:N	2.25	0.70
1:A:165:THR:OG1	1:A:165:THR:O	2.04	0.70
1:D:264:THR:OG1	1:D:266:ASN:ND2	2.24	0.70
1:A:234:THR:O	1:A:236:THR:N	2.24	0.70
1:A:69:THR:OG1	1:A:87:GLU:O	2.09	0.69
1:C:156:SER:O	1:C:156:SER:OG	2.08	0.69
1:B:305:ARG:NH2	1:B:327:GLU:OE1	2.25	0.69
1:C:264:THR:OG1	1:C:266:ASN:ND2	2.26	0.69
1:B:308:GLU:O	1:B:320:LYS:N	2.26	0.69
1:A:178:THR:OG1	1:A:178:THR:O	2.04	0.68
1:D:315:PHE:O	1:D:317:THR:N	2.26	0.68
1:D:178:THR:OG1	1:D:178:THR:O	2.06	0.68
1:B:165:THR:OG1	1:B:165:THR:O	2.08	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:LYS:N	1:B:63:GLN:NE2	2.41	0.68
1:B:325:GLU:OE2	1:B:326:GLY:N	2.27	0.68
1:D:234:THR:O	1:D:234:THR:OG1	2.12	0.67
1:A:175:SER:OG	1:A:176:ASN:N	2.24	0.66
1:D:281:ASN:OD1	1:D:315:PHE:CD2	2.49	0.66
1:B:234:THR:O	1:B:236:THR:N	2.29	0.66
1:A:214:THR:OG1	1:A:215:ILE:N	2.27	0.66
1:C:69:THR:OG1	1:C:87:GLU:O	2.13	0.65
1:A:264:THR:OG1	1:A:266:ASN:ND2	2.28	0.65
1:B:239:ASP:N	1:B:239:ASP:OD2	2.29	0.65
1:B:325:GLU:O	1:B:327:GLU:N	2.30	0.65
1:A:266:ASN:OD1	1:A:266:ASN:N	2.27	0.65
1:C:266:ASN:OD1	1:C:266:ASN:N	2.29	0.65
1:A:109:GLU:OE2	1:B:125:LYS:NZ	2.29	0.65
1:B:72:TYR:N	1:B:85:LEU:O	2.29	0.65
1:B:168:SER:O	1:B:170:GLY:N	2.29	0.65
1:A:173:VAL:CG2	1:A:174:ASN:N	2.60	0.64
1:C:165:THR:OG1	1:C:165:THR:O	2.12	0.64
1:B:69:THR:OG1	1:B:87:GLU:O	2.15	0.64
1:B:266:ASN:N	1:B:266:ASN:OD1	2.31	0.63
1:D:278:PHE:CE2	1:D:316:GLN:O	2.52	0.63
1:D:36:GLU:OE1	1:D:38:LYS:NZ	2.33	0.61
1:B:81:LYS:O	1:B:83:ASP:N	2.33	0.61
1:C:305:ARG:O	1:C:305:ARG:NH1	2.34	0.61
1:B:82:GLY:O	1:B:155:THR:OG1	2.18	0.61
1:D:311:VAL:N	1:D:318:GLU:OE1	2.34	0.61
1:D:69:THR:OG1	1:D:87:GLU:O	2.18	0.61
1:D:57:THR:OG1	1:D:57:THR:O	2.12	0.61
1:B:278:PHE:CE2	1:B:316:GLN:O	2.55	0.59
1:D:34:THR:OG1	1:D:326:GLY:O	2.19	0.59
1:A:239:ASP:N	1:A:239:ASP:OD2	2.36	0.59
1:B:174:ASN:OD1	1:B:174:ASN:C	2.42	0.58
1:B:234:THR:O	1:B:237:ILE:N	2.36	0.58
1:A:278:PHE:CE2	1:A:316:GLN:O	2.57	0.58
1:B:173:VAL:CG2	1:B:174:ASN:N	2.67	0.57
1:C:109:GLU:OE2	1:D:125:LYS:NZ	2.37	0.57
1:A:181:THR:OG1	1:A:182:ILE:N	2.35	0.57
1:C:281:ASN:OD1	1:C:315:PHE:O	2.22	0.57
1:C:168:SER:O	1:C:170:GLY:N	2.38	0.57
1:B:214:THR:OG1	1:B:215:ILE:N	2.37	0.57
1:B:147:ILE:O	1:B:150:ARG:N	2.39	0.56
1:D:290:LYS:NZ	1:D:290:LYS:O	2.39	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:173:VAL:CG2	1:C:174:ASN:N	2.69	0.56
1:D:266:ASN:OD1	1:D:266:ASN:N	2.39	0.56
1:D:173:VAL:CG2	1:D:174:ASN:N	2.69	0.56
1:A:156:SER:O	1:A:156:SER:OG	2.23	0.55
1:A:168:SER:O	1:A:170:GLY:N	2.39	0.55
1:A:178:THR:O	1:A:179:THR:C	2.43	0.55
1:C:228:ASP:OD2	1:C:229:SER:OG	2.23	0.55
1:B:219:ASN:OD1	1:B:220:LYS:NZ	2.40	0.55
1:B:191:MSE:O	1:B:251:VAL:N	2.39	0.54
1:C:234:THR:O	1:C:237:ILE:N	2.40	0.54
1:D:214:THR:OG1	1:D:215:ILE:N	2.40	0.54
1:A:217:SER:OG	1:B:199:GLU:O	2.25	0.54
1:A:191:MSE:O	1:A:251:VAL:N	2.41	0.54
1:B:102:ALA:O	1:B:105:ALA:N	2.40	0.54
1:A:228:ASP:OD2	1:A:229:SER:OG	2.26	0.54
1:C:219:ASN:OD1	1:C:220:LYS:NZ	2.40	0.54
1:D:219:ASN:OD1	1:D:220:LYS:NZ	2.40	0.53
1:D:72:TYR:N	1:D:85:LEU:O	2.41	0.53
1:D:168:SER:O	1:D:170:GLY:N	2.40	0.53
1:C:309:ILE:O	1:C:320:LYS:NZ	2.42	0.53
1:A:234:THR:O	1:A:237:ILE:N	2.42	0.53
1:D:228:ASP:OD2	1:D:229:SER:OG	2.25	0.53
1:B:164:SER:OG	1:B:165:THR:N	2.42	0.53
1:D:82:GLY:O	1:D:155:THR:OG1	2.27	0.53
1:B:228:ASP:OD2	1:B:229:SER:OG	2.26	0.52
1:A:147:ILE:O	1:A:150:ARG:N	2.42	0.52
1:A:327:GLU:OE1	1:A:328:LYS:NZ	2.42	0.52
1:B:175:SER:OG	1:B:176:ASN:N	2.40	0.52
1:C:289:ASP:N	1:C:289:ASP:OD1	2.42	0.52
1:C:248:ASN:OD1	1:C:248:ASN:N	2.42	0.52
1:A:72:TYR:N	1:A:85:LEU:O	2.43	0.51
1:C:97:TYR:OH	1:C:146:ARG:NH1	2.43	0.51
1:B:50:GLY:O	1:B:264:THR:N	2.43	0.51
1:B:102:ALA:O	1:B:104:LEU:N	2.44	0.51
1:B:305:ARG:NH1	1:B:327:GLU:OE2	2.44	0.51
1:C:147:ILE:O	1:C:150:ARG:N	2.44	0.51
1:B:181:THR:OG1	1:B:182:ILE:N	2.44	0.51
1:B:197:ILE:CG1	1:B:198:SER:N	2.73	0.51
1:A:315:PHE:N	1:A:316:GLN:OE1	2.44	0.51
1:C:214:THR:OG1	1:C:215:ILE:N	2.43	0.51
1:C:193:ILE:N	1:C:249:ILE:O	2.44	0.50
1:A:219:ASN:OD1	1:A:220:LYS:NZ	2.43	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:50:GLY:N	1:A:264:THR:O	2.45	0.50
1:C:81:LYS:O	1:C:83:ASP:N	2.44	0.50
1:B:234:THR:OG1	1:B:234:THR:O	2.29	0.49
1:A:106:SER:OG	1:A:107:THR:N	2.45	0.49
1:B:174:ASN:OD1	1:B:175:SER:O	2.30	0.49
1:D:178:THR:O	1:D:179:THR:C	2.50	0.49
1:B:103:ASN:OD1	1:B:138:SER:OG	2.31	0.49
1:C:102:ALA:O	1:C:105:ALA:N	2.46	0.48
1:D:50:GLY:O	1:D:264:THR:N	2.47	0.48
1:A:197:ILE:CG1	1:A:198:SER:N	2.75	0.48
1:C:281:ASN:ND2	1:C:284:VAL:CG2	2.77	0.48
1:B:237:ILE:C	1:B:238:SER:O	2.49	0.48
1:A:256:HIS:O	1:A:258:LEU:O	2.32	0.48
1:A:255:GLU:O	1:A:256:HIS:ND1	2.47	0.48
1:A:174:ASN:OD1	1:A:174:ASN:O	2.31	0.47
1:A:278:PHE:CD2	1:A:317:THR:O	2.67	0.47
1:A:102:ALA:O	1:A:105:ALA:N	2.47	0.47
1:C:82:GLY:O	1:C:155:THR:OG1	2.32	0.47
1:D:234:THR:OG1	1:D:236:THR:OG1	2.32	0.47
1:C:50:GLY:O	1:C:264:THR:N	2.47	0.47
1:D:34:THR:OG1	1:D:327:GLU:O	2.33	0.47
1:B:70:LYS:O	1:B:86:ALA:O	2.33	0.47
1:D:248:ASN:N	1:D:248:ASN:OD1	2.47	0.47
1:D:103:ASN:OD1	1:D:138:SER:OG	2.33	0.47
1:D:191:MSE:O	1:D:251:VAL:N	2.48	0.47
1:C:79:VAL:O	1:C:160:GLY:N	2.48	0.47
1:D:193:ILE:N	1:D:249:ILE:O	2.49	0.46
1:C:72:TYR:N	1:C:85:LEU:O	2.48	0.46
1:A:82:GLY:O	1:A:155:THR:OG1	2.34	0.46
1:B:50:GLY:N	1:B:264:THR:O	2.49	0.46
1:B:163:ILE:CG2	1:B:164:SER:N	2.78	0.46
1:B:106:SER:OG	1:B:107:THR:N	2.48	0.46
1:C:191:MSE:O	1:C:251:VAL:N	2.49	0.46
1:A:57:THR:O	1:A:57:THR:OG1	2.31	0.45
1:C:151:TYR:O	1:C:152:THR:C	2.54	0.45
1:B:202:ILE:O	1:B:204:LYS:O	2.34	0.45
1:D:79:VAL:O	1:D:160:GLY:N	2.49	0.45
1:B:76:GLY:N	1:B:162:VAL:O	2.49	0.45
1:D:102:ALA:O	1:D:105:ALA:N	2.50	0.45
1:B:151:TYR:O	1:B:152:THR:C	2.55	0.45
1:D:317:THR:CG2	1:D:318:GLU:N	2.80	0.45
1:D:197:ILE:CG1	1:D:198:SER:N	2.79	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:214:THR:O	1:D:265:GLU:N	2.50	0.45
1:D:97:TYR:OH	1:D:146:ARG:NH1	2.50	0.44
1:A:193:ILE:N	1:A:249:ILE:O	2.50	0.44
1:D:234:THR:O	1:D:237:ILE:N	2.50	0.44
1:C:315:PHE:O	1:C:316:GLN:O	2.36	0.44
1:D:289:ASP:OD1	1:D:289:ASP:N	2.49	0.44
1:C:324:THR:OG1	1:C:325:GLU:N	2.49	0.44
1:C:234:THR:OG1	1:C:236:THR:OG1	2.36	0.44
1:A:214:THR:O	1:A:265:GLU:N	2.51	0.44
1:D:278:PHE:CE2	1:D:316:GLN:CB	3.01	0.44
1:D:315:PHE:N	1:D:316:GLN:OE1	2.50	0.44
1:C:283:ALA:O	1:C:291:TYR:CG	2.71	0.44
1:A:86:ALA:CB	1:A:154:ILE:CB	2.96	0.44
1:A:174:ASN:OD1	1:A:174:ASN:C	2.57	0.44
1:A:175:SER:OG	1:A:176:ASN:O	2.36	0.44
1:A:214:THR:N	1:A:265:GLU:O	2.51	0.44
1:C:57:THR:OG1	1:C:57:THR:O	2.32	0.44
1:A:81:LYS:O	1:A:83:ASP:N	2.50	0.44
1:A:178:THR:O	1:A:180:PRO:CD	2.66	0.43
1:B:324:THR:OG1	1:B:325:GLU:N	2.52	0.43
1:D:314:ASP:OD1	1:D:316:GLN:NE2	2.51	0.43
1:C:202:ILE:O	1:C:204:LYS:O	2.37	0.43
1:C:76:GLY:N	1:C:162:VAL:O	2.52	0.43
1:C:156:SER:O	1:C:158:ILE:N	2.52	0.43
1:A:156:SER:O	1:A:158:ILE:N	2.52	0.43
1:B:248:ASN:N	1:B:248:ASN:OD1	2.51	0.43
1:A:97:TYR:OH	1:A:146:ARG:NH1	2.52	0.43
1:D:156:SER:O	1:D:158:ILE:N	2.52	0.43
1:C:327:GLU:O	1:C:329:VAL:N	2.52	0.43
1:C:235:THR:CB	1:C:246:TYR:CE1	3.01	0.43
1:B:238:SER:O	1:B:239:ASP:C	2.56	0.43
1:B:304:GLU:O	1:B:305:ARG:NH2	2.52	0.42
1:D:174:ASN:OD1	1:D:174:ASN:C	2.57	0.42
1:A:56:ASN:O	1:A:187:ASP:N	2.52	0.42
1:A:79:VAL:O	1:A:160:GLY:N	2.52	0.42
1:C:161:THR:N	1:C:186:ALA:O	2.52	0.42
1:B:40:GLY:O	1:B:275:ASN:N	2.52	0.42
1:A:52:ILE:O	1:A:260:ILE:O	2.38	0.42
1:C:171:GLN:O	1:C:173:VAL:N	2.53	0.42
1:C:56:ASN:O	1:C:187:ASP:N	2.53	0.42
1:B:156:SER:O	1:B:158:ILE:N	2.52	0.42
1:A:70:LYS:O	1:A:86:ALA:O	2.38	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:SER:O	1:A:200:GLY:N	2.53	0.42
1:C:174:ASN:C	1:C:174:ASN:OD1	2.57	0.42
1:B:182:ILE:O	1:B:183:ILE:CD1	2.68	0.42
1:A:64:VAL:CG2	1:A:65:SER:N	2.83	0.42
1:C:59:ASP:OD1	1:C:59:ASP:N	2.53	0.42
1:C:70:LYS:O	1:C:86:ALA:O	2.37	0.42
1:D:235:THR:CB	1:D:246:TYR:CE1	3.03	0.42
1:A:74:LYS:O	1:A:76:GLY:N	2.52	0.42
1:B:204:LYS:O	1:B:205:VAL:CG2	2.68	0.41
1:B:79:VAL:O	1:B:160:GLY:N	2.53	0.41
1:B:147:ILE:O	1:B:149:LEU:N	2.53	0.41
1:C:177:GLN:NE2	1:D:177:GLN:NE2	2.68	0.41
1:D:279:ILE:O	1:D:280:PRO:C	2.58	0.41
1:C:238:SER:O	1:C:239:ASP:C	2.58	0.41
1:B:68:ILE:CD1	1:B:69:THR:N	2.84	0.41
1:C:197:ILE:CG1	1:C:198:SER:N	2.83	0.41
1:C:178:THR:O	1:C:179:THR:C	2.58	0.41
1:B:165:THR:N	1:B:166:PRO:CD	2.82	0.41
1:A:50:GLY:O	1:A:264:THR:N	2.54	0.41
1:C:214:THR:O	1:C:265:GLU:N	2.53	0.41
1:A:151:TYR:O	1:A:152:THR:C	2.60	0.41
1:A:147:ILE:CG2	1:A:148:ASN:N	2.84	0.40
1:A:171:GLN:O	1:A:173:VAL:N	2.54	0.40
1:D:147:ILE:O	1:D:150:ARG:N	2.55	0.40
1:C:117:LEU:O	1:C:119:ALA:N	2.54	0.40
1:D:81:LYS:O	1:D:83:ASP:N	2.53	0.40
1:A:213:PHE:CE2	1:A:223:TYR:CB	3.05	0.40
1:B:213:PHE:CE2	1:B:223:TYR:CB	3.04	0.40
1:A:182:ILE:O	1:A:183:ILE:CD1	2.70	0.40
1:D:52:ILE:O	1:D:260:ILE:O	2.39	0.40
1:B:235:THR:CB	1:B:246:TYR:CE1	3.05	0.40

All (3) 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	Distance(Å)	Clash(Å)
1:C:176:ASN:O	1:D:174:ASN:ND2[3_565]	1.97	0.23
1:A:199:GLU:O	1:B:217:SER:OG[2_665]	2.11	0.09
1:A:176:ASN:O	1:B:174:ASN:ND2[2_665]	2.12	0.08

## 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	270/341 (79%)	163 (60%)	51 (19%)	56 (21%)	0	2
1	B	277/341 (81%)	170 (61%)	56 (20%)	51 (18%)	0	3
1	C	270/341 (79%)	164 (61%)	49 (18%)	57 (21%)	0	2
1	D	270/341 (79%)	161 (60%)	59 (22%)	50 (18%)	0	3
All	All	1087/1364 (80%)	658 (60%)	215 (20%)	214 (20%)	0	2

All (214) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	75	LEU
1	A	82	GLY
1	A	121	GLN
1	A	122	ALA
1	A	124	SER
1	A	152	THR
1	A	169	GLU
1	A	190	LYS
1	A	196	GLU
1	A	215	ILE
1	A	216	LEU
1	A	232	PRO
1	A	235	THR
1	A	238	SER
1	A	242	ALA
1	A	257	VAL
1	A	281	ASN
1	A	309	ILE
1	A	317	THR
1	B	81	LYS
1	B	82	GLY
1	B	121	GLN
1	B	122	ALA

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Mol	Chain	Res	Type
1	B	124	SER
1	B	152	THR
1	B	169	GLU
1	B	173	VAL
1	B	190	LYS
1	B	196	GLU
1	B	215	ILE
1	B	216	LEU
1	B	232	PRO
1	B	235	THR
1	B	257	VAL
1	B	281	ASN
1	B	317	THR
1	B	323	LEU
1	B	326	GLY
1	B	327	GLU
1	B	331	ILE
1	C	82	GLY
1	C	121	GLN
1	C	122	ALA
1	C	124	SER
1	C	151	TYR
1	C	152	THR
1	C	169	GLU
1	C	173	VAL
1	C	196	GLU
1	C	216	LEU
1	C	232	PRO
1	C	235	THR
1	C	238	SER
1	C	258	LEU
1	C	281	ASN
1	C	282	LEU
1	C	307	ILE
1	C	308	GLU
1	C	316	GLN
1	C	323	LEU
1	C	328	LYS
1	C	329	VAL
1	D	82	GLY
1	D	121	GLN
1	D	122	ALA

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Mol	Chain	Res	Type
1	D	124	SER
1	D	152	THR
1	D	169	GLU
1	D	173	VAL
1	D	196	GLU
1	D	215	ILE
1	D	216	LEU
1	D	232	PRO
1	D	235	THR
1	D	238	SER
1	D	258	LEU
1	D	281	ASN
1	D	282	LEU
1	D	316	GLN
1	D	317	THR
1	A	45	ASN
1	A	103	ASN
1	A	114	TYR
1	A	151	TYR
1	A	258	LEU
1	A	329	VAL
1	B	45	ASN
1	B	66	GLY
1	B	83	ASP
1	B	103	ASN
1	B	114	TYR
1	B	151	TYR
1	B	182	ILE
1	B	246	TYR
1	B	275	ASN
1	C	45	ASN
1	C	103	ASN
1	C	114	TYR
1	C	182	ILE
1	C	190	LYS
1	C	215	ILE
1	C	246	TYR
1	C	262	MSE
1	C	269	LYS
1	C	310	GLY
1	D	45	ASN
1	D	103	ASN

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Mol	Chain	Res	Type
1	D	182	ILE
1	D	190	LYS
1	D	257	VAL
1	D	269	LYS
1	A	81	LYS
1	A	95	ALA
1	A	106	SER
1	A	140	ALA
1	A	141	ALA
1	A	222	VAL
1	A	269	LYS
1	A	275	ASN
1	A	282	LEU
1	B	86	ALA
1	B	87	GLU
1	B	95	ALA
1	B	106	SER
1	B	140	ALA
1	B	205	VAL
1	B	258	LEU
1	C	83	ASP
1	C	86	ALA
1	C	148	ASN
1	C	257	VAL
1	C	306	GLU
1	C	331	ILE
1	D	66	GLY
1	D	81	LYS
1	D	86	ALA
1	D	106	SER
1	D	151	TYR
1	D	222	VAL
1	D	262	MSE
1	D	275	ASN
1	D	321	SER
1	A	76	GLY
1	A	83	ASP
1	A	110	GLN
1	A	148	ASN
1	A	155	THR
1	A	173	VAL
1	A	182	ILE

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Mol	Chain	Res	Type
1	B	222	VAL
1	B	269	LYS
1	C	81	LYS
1	C	106	SER
1	C	197	ILE
1	C	205	VAL
1	C	222	VAL
1	C	275	ASN
1	C	327	GLU
1	D	87	GLU
1	D	140	ALA
1	D	205	VAL
1	D	234	THR
1	D	246	TYR
1	D	327	GLU
1	A	36	GLU
1	A	87	GLU
1	A	170	GLY
1	A	205	VAL
1	A	221	THR
1	A	234	THR
1	B	110	GLN
1	B	155	THR
1	B	170	GLY
1	B	230	VAL
1	B	313	ASN
1	C	118	VAL
1	C	140	ALA
1	C	155	THR
1	C	157	PRO
1	C	170	GLY
1	C	221	THR
1	D	114	TYR
1	D	155	THR
1	D	197	ILE
1	A	66	GLY
1	A	118	VAL
1	A	176	ASN
1	B	118	VAL
1	C	66	GLY
1	C	87	GLU
1	D	118	VAL

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Mol	Chain	Res	Type
1	D	170	GLY
1	D	230	VAL
1	A	40	GLY
1	A	230	VAL
1	D	157	PRO
1	D	251	VAL
1	A	276	VAL
1	C	64	VAL
1	C	276	VAL
1	D	64	VAL
1	D	276	VAL
1	D	284	VAL
1	A	64	VAL
1	A	197	ILE
1	C	251	VAL
1	B	64	VAL
1	B	157	PRO
1	B	253	ASN
1	B	276	VAL
1	B	329	VAL
1	C	230	VAL
1	B	37	VAL

### 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	236/288 (82%)	132 (56%)	104 (44%)	0	1
1	B	245/288 (85%)	134 (55%)	111 (45%)	0	0
1	C	239/288 (83%)	141 (59%)	98 (41%)	0	1
1	D	238/288 (83%)	134 (56%)	104 (44%)	0	1
All	All	958/1152 (83%)	541 (56%)	417 (44%)	0	1

All (417) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	THR
1	A	35	GLU
1	A	37	VAL
1	A	38	LYS
1	A	39	ARG
1	A	41	ASN
1	A	42	ILE
1	A	44	LYS
1	A	49	THR
1	A	52	ILE
1	A	56	ASN
1	A	58	VAL
1	A	67	LYS
1	A	68	ILE
1	A	69	THR
1	A	75	LEU
1	A	80	LYS
1	A	81	LYS
1	A	84	LEU
1	A	85	LEU
1	A	89	ASP
1	A	92	THR
1	A	97	TYR
1	A	101	GLN
1	A	106	SER
1	A	107	THR
1	A	109	GLU
1	A	113	ARG
1	A	116	LEU
1	A	125	LYS
1	A	127	GLN
1	A	128	TYR
1	A	130	ASP
1	A	136	LEU
1	A	139	LYS
1	A	146	ARG
1	A	147	ILE
1	A	149	LEU
1	A	150	ARG
1	A	152	THR
1	A	153	LYS
1	A	155	THR
1	A	156	SER

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Mol	Chain	Res	Type
1	A	161	THR
1	A	163	ILE
1	A	167	VAL
1	A	173	VAL
1	A	174	ASN
1	A	176	ASN
1	A	177	GLN
1	A	180	PRO
1	A	181	THR
1	A	182	ILE
1	A	183	ILE
1	A	185	VAL
1	A	188	LEU
1	A	191	MSE
1	A	192	ARG
1	A	197	ILE
1	A	198	SER
1	A	201	ASP
1	A	202	ILE
1	A	203	THR
1	A	204	LYS
1	A	205	VAL
1	A	206	LYS
1	A	210	ASP
1	A	212	THR
1	A	215	ILE
1	A	216	LEU
1	A	220	LYS
1	A	221	THR
1	A	224	HIS
1	A	227	ILE
1	A	228	ASP
1	A	229	SER
1	A	234	THR
1	A	235	THR
1	A	236	THR
1	A	237	ILE
1	A	239	ASP
1	A	241	SER
1	A	248	ASN
1	A	250	ILE
1	A	251	VAL

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Mol	Chain	Res	Type
1	A	252	GLU
1	A	256	HIS
1	A	258	LEU
1	A	259	ARG
1	A	260	ILE
1	A	263	THR
1	A	266	ASN
1	A	267	ASN
1	A	268	ILE
1	A	270	ILE
1	A	273	VAL
1	A	276	VAL
1	A	277	LEU
1	A	309	ILE
1	A	311	VAL
1	A	312	GLN
1	A	317	THR
1	A	327	GLU
1	A	329	VAL
1	B	34	THR
1	B	35	GLU
1	B	36	GLU
1	B	37	VAL
1	B	41	ASN
1	B	42	ILE
1	B	44	LYS
1	B	49	THR
1	B	52	ILE
1	B	56	ASN
1	B	58	VAL
1	B	67	LYS
1	B	68	ILE
1	B	69	THR
1	B	74	LYS
1	B	75	LEU
1	B	80	LYS
1	B	81	LYS
1	B	84	LEU
1	B	89	ASP
1	B	92	THR
1	B	97	TYR
1	B	101	GLN

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Mol	Chain	Res	Type
1	B	106	SER
1	B	107	THR
1	B	109	GLU
1	B	113	ARG
1	B	116	LEU
1	B	125	LYS
1	B	127	GLN
1	B	128	TYR
1	B	130	ASP
1	B	136	LEU
1	B	139	LYS
1	B	144	GLN
1	B	146	ARG
1	B	147	ILE
1	B	150	ARG
1	B	152	THR
1	B	153	LYS
1	B	155	THR
1	B	156	SER
1	B	161	THR
1	B	163	ILE
1	B	167	VAL
1	B	173	VAL
1	B	174	ASN
1	B	176	ASN
1	B	177	GLN
1	B	180	PRO
1	B	181	THR
1	B	182	ILE
1	B	183	ILE
1	B	185	VAL
1	B	188	LEU
1	B	189	SER
1	B	192	ARG
1	B	197	ILE
1	B	198	SER
1	B	201	ASP
1	B	202	ILE
1	B	203	THR
1	B	204	LYS
1	B	205	VAL
1	B	206	LYS

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Mol	Chain	Res	Type
1	B	210	ASP
1	B	212	THR
1	B	215	ILE
1	B	216	LEU
1	B	220	LYS
1	B	221	THR
1	B	224	HIS
1	B	228	ASP
1	B	229	SER
1	B	234	THR
1	B	235	THR
1	B	236	THR
1	B	237	ILE
1	B	239	ASP
1	B	248	ASN
1	B	250	ILE
1	B	251	VAL
1	B	252	GLU
1	B	256	HIS
1	B	258	LEU
1	B	259	ARG
1	B	260	ILE
1	B	263	THR
1	B	266	ASN
1	B	267	ASN
1	B	268	ILE
1	B	270	ILE
1	B	273	VAL
1	B	276	VAL
1	B	277	LEU
1	B	288	GLN
1	B	291	TYR
1	B	292	VAL
1	B	304	GLU
1	B	305	ARG
1	B	309	ILE
1	B	311	VAL
1	B	312	GLN
1	B	315	PHE
1	B	319	VAL
1	B	320	LYS
1	B	321	SER

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Mol	Chain	Res	Type
1	B	323	LEU
1	B	325	GLU
1	B	329	VAL
1	B	331	ILE
1	C	41	ASN
1	C	42	ILE
1	C	44	LYS
1	C	49	THR
1	C	52	ILE
1	C	56	ASN
1	C	58	VAL
1	C	67	LYS
1	C	68	ILE
1	C	69	THR
1	C	74	LYS
1	C	75	LEU
1	C	80	LYS
1	C	81	LYS
1	C	84	LEU
1	C	89	ASP
1	C	92	THR
1	C	97	TYR
1	C	101	GLN
1	C	106	SER
1	C	109	GLU
1	C	113	ARG
1	C	116	LEU
1	C	121	GLN
1	C	125	LYS
1	C	127	GLN
1	C	130	ASP
1	C	132	ASN
1	C	136	LEU
1	C	139	LYS
1	C	146	ARG
1	C	147	ILE
1	C	150	ARG
1	C	152	THR
1	C	153	LYS
1	C	155	THR
1	C	156	SER
1	C	161	THR

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Mol	Chain	Res	Type
1	C	163	ILE
1	C	167	VAL
1	C	173	VAL
1	C	174	ASN
1	C	176	ASN
1	C	177	GLN
1	C	180	PRO
1	C	181	THR
1	C	182	ILE
1	C	183	ILE
1	C	188	LEU
1	C	192	ARG
1	C	197	ILE
1	C	198	SER
1	C	201	ASP
1	C	202	ILE
1	C	204	LYS
1	C	205	VAL
1	C	206	LYS
1	C	210	ASP
1	C	212	THR
1	C	215	ILE
1	C	216	LEU
1	C	220	LYS
1	C	224	HIS
1	C	228	ASP
1	C	229	SER
1	C	234	THR
1	C	235	THR
1	C	236	THR
1	C	237	ILE
1	C	239	ASP
1	C	248	ASN
1	C	250	ILE
1	C	251	VAL
1	C	252	GLU
1	C	258	LEU
1	C	259	ARG
1	C	260	ILE
1	C	263	THR
1	C	266	ASN
1	C	267	ASN

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Mol	Chain	Res	Type
1	C	268	ILE
1	C	270	ILE
1	C	273	VAL
1	C	276	VAL
1	C	277	LEU
1	C	284	VAL
1	C	289	ASP
1	C	290	LYS
1	C	293	VAL
1	C	305	ARG
1	C	307	ILE
1	C	308	GLU
1	C	315	PHE
1	C	318	GLU
1	C	320	LYS
1	C	323	LEU
1	C	325	GLU
1	C	327	GLU
1	D	34	THR
1	D	36	GLU
1	D	37	VAL
1	D	42	ILE
1	D	44	LYS
1	D	49	THR
1	D	52	ILE
1	D	56	ASN
1	D	58	VAL
1	D	67	LYS
1	D	68	ILE
1	D	69	THR
1	D	74	LYS
1	D	80	LYS
1	D	81	LYS
1	D	84	LEU
1	D	89	ASP
1	D	92	THR
1	D	97	TYR
1	D	101	GLN
1	D	106	SER
1	D	109	GLU
1	D	113	ARG
1	D	116	LEU

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Mol	Chain	Res	Type
1	D	121	GLN
1	D	125	LYS
1	D	127	GLN
1	D	130	ASP
1	D	136	LEU
1	D	139	LYS
1	D	146	ARG
1	D	147	ILE
1	D	149	LEU
1	D	150	ARG
1	D	152	THR
1	D	153	LYS
1	D	155	THR
1	D	156	SER
1	D	161	THR
1	D	163	ILE
1	D	167	VAL
1	D	173	VAL
1	D	174	ASN
1	D	176	ASN
1	D	177	GLN
1	D	180	PRO
1	D	181	THR
1	D	182	ILE
1	D	183	ILE
1	D	185	VAL
1	D	188	LEU
1	D	192	ARG
1	D	193	ILE
1	D	197	ILE
1	D	198	SER
1	D	201	ASP
1	D	202	ILE
1	D	203	THR
1	D	204	LYS
1	D	205	VAL
1	D	206	LYS
1	D	210	ASP
1	D	212	THR
1	D	215	ILE
1	D	216	LEU
1	D	220	LYS

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Mol	Chain	Res	Type
1	D	221	THR
1	D	224	HIS
1	D	228	ASP
1	D	229	SER
1	D	231	ASP
1	D	234	THR
1	D	235	THR
1	D	236	THR
1	D	237	ILE
1	D	239	ASP
1	D	248	ASN
1	D	250	ILE
1	D	251	VAL
1	D	252	GLU
1	D	256	HIS
1	D	258	LEU
1	D	259	ARG
1	D	260	ILE
1	D	263	THR
1	D	266	ASN
1	D	267	ASN
1	D	268	ILE
1	D	270	ILE
1	D	273	VAL
1	D	276	VAL
1	D	277	LEU
1	D	281	ASN
1	D	284	VAL
1	D	288	GLN
1	D	290	LYS
1	D	292	VAL
1	D	307	ILE
1	D	311	VAL
1	D	312	GLN
1	D	315	PHE
1	D	319	VAL
1	D	320	LYS
1	D	324	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

There are no ligands in this entry.

### 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	276/341 (80%)	-0.38	1 (0%) 90 71	7, 60, 178, 245	1 (0%)
1	B	285/341 (83%)	-0.35	0 100 100	7, 63, 166, 285	1 (0%)
1	C	278/341 (81%)	-0.37	0 100 100	27, 98, 200, 277	1 (0%)
1	D	278/341 (81%)	-0.36	1 (0%) 90 71	27, 93, 190, 275	1 (0%)
All	All	1117/1364 (81%)	-0.36	2 (0%) 93 80	7, 81, 185, 285	4 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	GLU	2.1
1	D	38	LYS	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

There are no ligands in this entry.

### 6.5 Other polymers

There are no such residues in this entry.