



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:33 pm GMT

PDB ID : 2OWL  
Title : Crystal structure of E. coli RdgC  
Authors : Briggs, G.S.; McEwan, P.A.; Yu, J.; Moore, T.; Emsley, J.; Lloyd, R.G.  
Deposited on : 2007-02-16  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

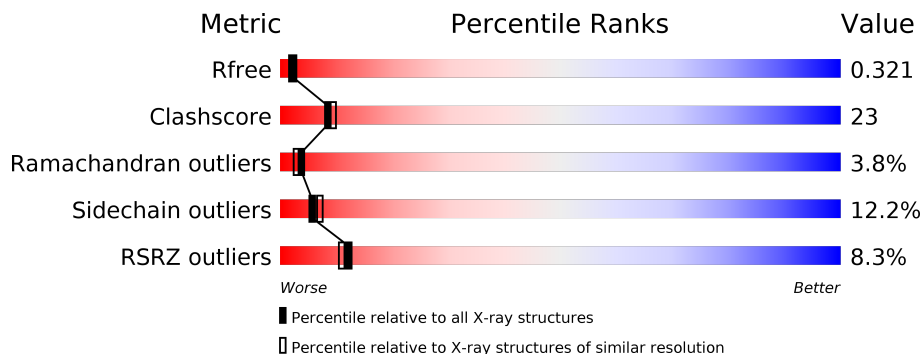
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


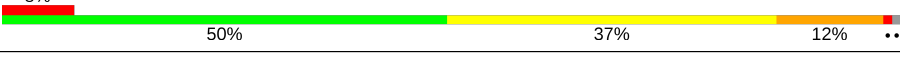
The reported resolution of this entry is 2.40 Å.

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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	303	
1	B	303	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4806 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 Recombination-associated protein rdgC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	Se	0	0	0
			2365	1489	406	452	5	13			
1	B	301	Total	C	N	O	S	Se	0	0	0
			2357	1484	405	451	5	12			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	8	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	23	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	30	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	40	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	43	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	49	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	127	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	128	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	138	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	168	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	244	MSE	MET	MODIFIED RESIDUE	UNP P36767
A	282	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	1	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	8	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	23	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	30	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	40	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	43	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	49	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	127	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	128	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	138	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	168	MSE	MET	MODIFIED RESIDUE	UNP P36767
B	244	MSE	MET	MODIFIED RESIDUE	UNP P36767

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	282	MSE	MET	MODIFIED RESIDUE	UNP P36767

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0

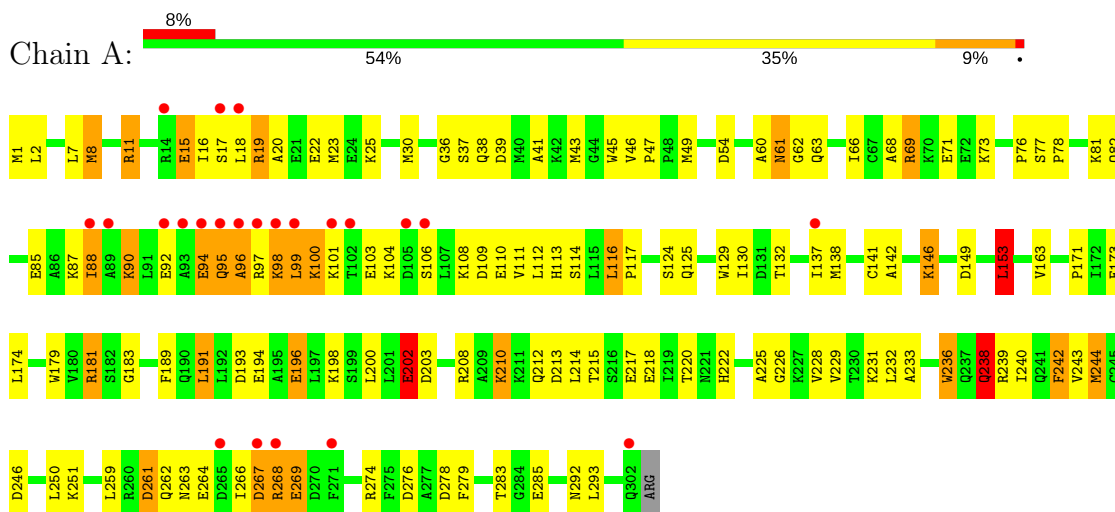
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	49	Total O 49 49	0	0
3	B	33	Total O 33 33	0	0

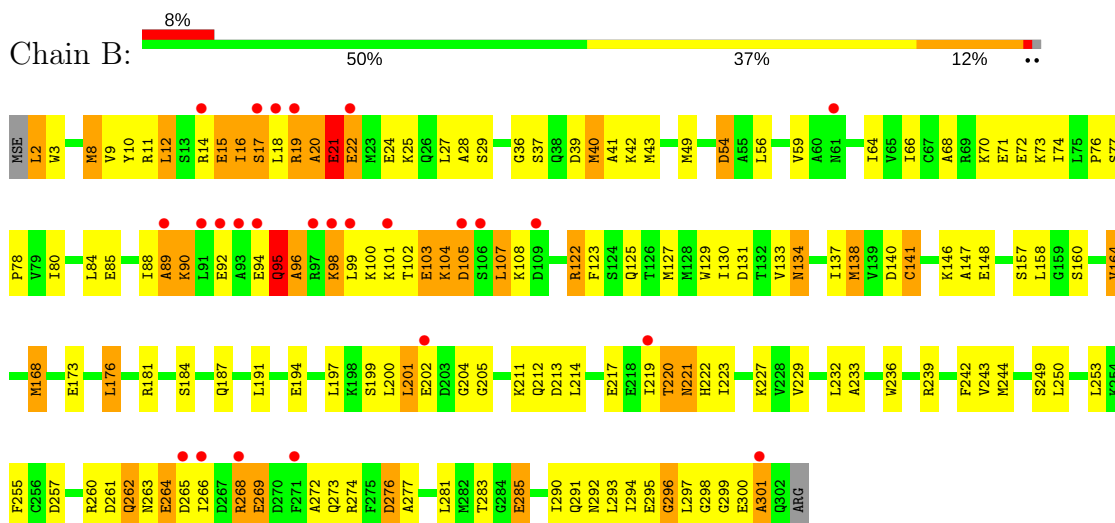
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Recombination-associated protein rdgC



#### • Molecule 1: Recombination-associated protein rdgC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.42Å 95.68Å 171.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.40 19.79 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.80-2.40) 98.2 (19.79-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.67 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.232 , 0.326 0.227 , 0.321	Depositor DCC
$R_{free}$ test set	3355 reflections (11.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.0	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

### 5.1 Standard geometry

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

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	1.57	19/2386 (0.8%)	1.39	26/3190 (0.8%)
1	B	1.43	16/2378 (0.7%)	1.29	9/3180 (0.3%)
All	All	1.50	35/4764 (0.7%)	1.34	35/6370 (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	B	0	4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	GLY	N-CA	10.31	1.61	1.46
1	A	90	LYS	CE-NZ	8.95	1.71	1.49
1	B	148	GLU	CG-CD	7.89	1.63	1.51
1	A	229	VAL	CA-CB	7.79	1.71	1.54
1	A	202	GLU	CG-CD	7.43	1.63	1.51
1	A	196	GLU	CG-CD	-7.20	1.41	1.51
1	B	301	ALA	CA-CB	7.16	1.67	1.52
1	A	141	CYS	CB-SG	-7.14	1.70	1.82
1	B	211	LYS	CD-CE	6.98	1.68	1.51
1	A	238	GLN	CB-CG	6.54	1.70	1.52
1	B	211	LYS	CE-NZ	6.29	1.64	1.49
1	B	291	GLN	CG-CD	6.22	1.65	1.51
1	B	10	TYR	CD1-CE1	6.07	1.48	1.39
1	A	179	TRP	CD2-CE2	5.95	1.48	1.41
1	A	233	ALA	CA-CB	-5.94	1.40	1.52
1	A	210	LYS	CD-CE	5.88	1.66	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	LYS	CE-NZ	5.82	1.63	1.49
1	B	148	GLU	CD-OE1	5.81	1.32	1.25
1	A	193	ASP	CB-CG	5.72	1.63	1.51
1	B	54	ASP	CB-CG	5.64	1.63	1.51
1	B	164	VAL	CA-CB	5.62	1.66	1.54
1	A	189	PHE	CG-CD1	-5.60	1.30	1.38
1	A	194	GLU	CD-OE1	5.60	1.31	1.25
1	B	22	GLU	CG-CD	5.53	1.60	1.51
1	B	141	CYS	CB-SG	-5.46	1.73	1.81
1	A	242	PHE	CE2-CZ	5.44	1.47	1.37
1	B	298	GLY	C-O	5.42	1.32	1.23
1	B	243	VAL	CA-CB	5.37	1.66	1.54
1	A	236	TRP	N-CA	-5.37	1.35	1.46
1	A	189	PHE	CD2-CE2	-5.33	1.28	1.39
1	A	153	LEU	CG-CD1	5.31	1.71	1.51
1	B	123	PHE	CE1-CZ	5.24	1.47	1.37
1	A	90	LYS	CD-CE	5.14	1.64	1.51
1	B	285	GLU	CB-CG	-5.10	1.42	1.52
1	B	173	GLU	CB-CG	-5.08	1.42	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	ASP	CB-CG-OD1	8.03	125.53	118.30
1	A	208	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	149	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	A	11	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	210	LYS	CD-CE-NZ	7.14	128.13	111.70
1	B	181	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	246	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	8	MSE	CG-SE-CE	6.73	113.71	98.90
1	A	181	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	240	ILE	CG1-CB-CG2	-6.67	96.73	111.40
1	A	153	LEU	CB-CG-CD2	6.36	121.81	111.00
1	B	213	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	54	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	261	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	B	27	LEU	CA-CB-CG	5.88	128.82	115.30
1	B	140	ASP	CB-CG-OD1	5.87	123.59	118.30
1	A	200	LEU	CB-CG-CD1	-5.81	101.12	111.00
1	A	11	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	A	225	ALA	C-N-CA	-5.80	110.12	122.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	MSE	CA-CB-CG	5.72	123.02	113.30
1	A	153	LEU	CA-CB-CG	5.70	128.42	115.30
1	A	243	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	A	251	LYS	CD-CE-NZ	-5.41	99.27	111.70
1	A	69	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	11	ARG	CG-CD-NE	-5.34	100.58	111.80
1	A	259	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	B	213	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	122	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	244	MSE	CG-SE-CE	5.18	110.31	98.90
1	A	90	LYS	CD-CE-NZ	-5.17	99.80	111.70
1	A	191	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	276	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	225	ALA	CA-C-N	5.08	126.37	116.20
1	A	214	LEU	N-CA-C	5.07	124.68	111.00
1	A	225	ALA	O-C-N	-5.06	114.59	123.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	17	SER	Peptide
1	B	264	GLU	Peptide
1	B	300	GLU	Peptide
1	B	95	GLN	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2365	0	2413	107	0
1	B	2357	0	2400	119	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	49	0	0	3	0
3	B	33	0	0	0	0
All	All	4806	0	4813	219	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 23.

All (219) 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:A:90:LYS:NZ	1:A:90:LYS:CE	1.71	1.53
1:A:244:MSE:CE	1:A:293:LEU:HD21	1.60	1.30
1:B:138:MSE:HE2	1:B:290:ILE:CD1	1.69	1.20
1:B:138:MSE:CE	1:B:290:ILE:HD13	1.81	1.09
1:A:244:MSE:HE3	1:A:293:LEU:HD11	1.29	1.07
1:B:268:ARG:HH11	1:B:268:ARG:HG3	1.14	1.04
1:A:244:MSE:HE3	1:A:293:LEU:CD1	1.87	1.03
1:B:138:MSE:HE2	1:B:290:ILE:HD13	1.36	1.00
1:A:244:MSE:HE1	1:A:293:LEU:HD21	1.01	0.99
1:B:138:MSE:HE2	1:B:290:ILE:HD11	1.41	0.99
1:A:244:MSE:CE	1:A:293:LEU:CD2	2.41	0.98
1:A:244:MSE:HE1	1:A:293:LEU:CD2	1.95	0.97
1:B:9:VAL:HG22	1:B:138:MSE:HE3	1.46	0.96
1:A:236:TRP:HE1	1:A:292:ASN:HD22	1.15	0.95
1:B:138:MSE:CE	1:B:290:ILE:CD1	2.43	0.94
1:A:7:LEU:HD11	1:A:138:MSE:HG3	1.50	0.93
1:B:102:THR:HA	1:B:105:ASP:HB3	1.50	0.91
1:A:263:ASN:HB3	1:A:266:ILE:HD13	1.52	0.90
1:A:222:HIS:HE1	1:B:222:HIS:HE1	1.18	0.89
1:A:244:MSE:HE3	1:A:293:LEU:HD21	1.61	0.82
1:B:236:TRP:HE1	1:B:292:ASN:HD22	1.26	0.81
1:B:129:TRP:CE3	1:B:138:MSE:HG3	2.15	0.81
1:B:242:PHE:HE2	1:B:244:MSE:CE	1.94	0.81
1:B:242:PHE:HE2	1:B:244:MSE:HE2	1.45	0.81
1:A:63:GLN:HE21	1:A:129:TRP:HE1	1.30	0.79
1:B:268:ARG:NH1	1:B:268:ARG:HG3	1.93	0.78
1:B:168:MSE:HE1	1:B:294:ILE:HA	1.66	0.78
1:A:99:LEU:HB3	1:A:100:LYS:HB2	1.64	0.78
1:B:138:MSE:HE1	1:B:290:ILE:HD13	1.66	0.78
1:B:236:TRP:HE1	1:B:292:ASN:ND2	1.82	0.77
1:B:39:ASP:O	1:B:40:MSE:HB3	1.85	0.77
1:B:261:ASP:O	1:B:264:GLU:HB2	1.84	0.77
1:A:69:ARG:HD2	1:A:125:GLN:HE21	1.51	0.76
1:B:104:LYS:HE3	1:B:108:LYS:HE2	1.69	0.75
1:B:8:MSE:HE3	1:B:249:SER:HB3	1.66	0.75
1:B:242:PHE:CE2	1:B:244:MSE:HE2	2.20	0.75
1:A:217:GLU:HA	1:A:220:THR:HB	1.69	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:TRP:CZ3	1:B:138:MSE:HG3	2.22	0.74
1:B:268:ARG:HH11	1:B:268:ARG:CG	1.98	0.74
1:A:244:MSE:HE3	1:A:293:LEU:CD2	2.14	0.74
1:B:39:ASP:O	1:B:40:MSE:CB	2.35	0.74
1:A:222:HIS:CE1	1:B:222:HIS:HE1	2.03	0.73
1:A:60:ALA:O	1:A:61:ASN:HB2	1.87	0.73
1:A:62:GLY:O	1:A:132:THR:OG1	2.05	0.72
1:B:242:PHE:CE2	1:B:244:MSE:CE	2.72	0.72
1:B:2:LEU:HD12	1:B:3:TRP:HD1	1.55	0.72
1:B:104:LYS:HD3	1:B:105:ASP:N	2.03	0.72
1:A:63:GLN:NE2	1:A:129:TRP:HE1	1.86	0.72
1:A:267:ASP:HB3	1:A:269:GLU:HG3	1.72	0.72
1:A:95:GLN:HA	1:A:95:GLN:HE21	1.53	0.72
1:A:222:HIS:HE1	1:B:222:HIS:CE1	2.07	0.71
1:B:85:GLU:HA	1:B:88:ILE:HG12	1.73	0.71
1:A:15:GLU:HG2	1:A:16:ILE:H	1.57	0.70
1:B:9:VAL:HG22	1:B:138:MSE:CE	2.22	0.69
1:A:7:LEU:HD11	1:A:138:MSE:CG	2.22	0.69
1:A:90:LYS:NZ	1:A:90:LYS:CD	2.56	0.69
1:A:15:GLU:HG2	1:A:16:ILE:N	2.08	0.68
1:A:110:GLU:O	1:A:114:SER:HB2	1.93	0.68
1:B:2:LEU:HD12	1:B:3:TRP:CD1	2.29	0.67
1:B:134:ASN:N	1:B:134:ASN:HD22	1.92	0.67
1:A:244:MSE:HE3	1:A:293:LEU:CG	2.25	0.67
1:A:183:GLY:HA2	1:A:215:THR:HG22	1.77	0.66
1:A:242:PHE:CE2	1:A:244:MSE:HE2	2.31	0.66
1:A:112:LEU:O	1:A:116:LEU:HB2	1.96	0.66
1:A:85:GLU:HA	1:A:88:ILE:HG22	1.78	0.65
1:A:94:GLU:HA	1:A:94:GLU:OE2	1.96	0.65
1:B:168:MSE:HE3	1:B:299:GLY:H	1.62	0.64
1:B:36:GLY:N	1:B:39:ASP:OD2	2.18	0.64
1:B:244:MSE:CE	1:B:293:LEU:HD21	2.28	0.64
1:A:41:ALA:HA	1:A:71:GLU:O	1.99	0.63
1:A:236:TRP:HE1	1:A:292:ASN:ND2	1.94	0.62
1:B:273:GLN:HA	1:B:276:ASP:OD2	1.98	0.62
1:B:214:LEU:HA	1:B:219:ILE:HG13	1.81	0.62
1:B:104:LYS:HE3	1:B:108:LYS:CE	2.29	0.62
1:B:88:ILE:HG13	1:B:89:ALA:N	2.13	0.62
1:A:130:ILE:HG12	1:A:137:ILE:HD13	1.80	0.62
1:A:1:MSE:HG2	1:A:2:LEU:N	2.15	0.62
1:A:238:GLN:HA	1:A:238:GLN:OE1	2.00	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ASP:O	1:A:73:LYS:NZ	2.27	0.60
1:A:98:LYS:HZ2	1:A:99:LEU:H	1.49	0.59
1:B:295:GLU:O	1:B:296:GLY:C	2.39	0.59
1:B:40:MSE:HE3	1:B:73:LYS:HB2	1.84	0.59
1:A:16:ILE:CD1	1:A:18:LEU:HB3	2.33	0.59
1:A:100:LYS:H	1:A:103:GLU:HB2	1.68	0.58
1:A:212:GLN:HG3	1:A:213:ASP:N	2.18	0.58
1:A:239:ARG:NE	1:A:285:GLU:OE2	2.32	0.58
1:B:168:MSE:CE	1:B:294:ILE:HA	2.34	0.58
1:B:88:ILE:HG13	1:B:89:ALA:H	1.67	0.58
1:A:76:PRO:HG2	1:B:74:ILE:HD13	1.87	0.57
1:A:38:GLN:HE22	1:A:113:HIS:HA	1.69	0.57
1:A:218:GLU:OE1	1:B:227:LYS:NZ	2.38	0.56
1:B:220:THR:HA	1:B:223:ILE:HD12	1.87	0.56
1:A:100:LYS:N	1:A:103:GLU:HG3	2.20	0.56
1:B:43:MSE:HB2	1:B:70:LYS:HD3	1.86	0.56
1:A:196:GLU:HB3	1:A:231:LYS:HB2	1.88	0.56
1:A:92:GLU:HG2	1:A:96:ALA:HA	1.87	0.56
1:B:272:ALA:O	1:B:276:ASP:OD2	2.23	0.55
1:B:244:MSE:HE1	1:B:293:LEU:HD21	1.87	0.55
1:B:168:MSE:HE2	1:B:297:LEU:HB2	1.89	0.55
1:A:7:LEU:HD23	1:A:250:LEU:HD22	1.89	0.54
1:A:202:GLU:O	1:A:203:ASP:HB2	2.08	0.54
1:B:141:CYS:SG	1:B:147:ALA:HB2	2.48	0.54
1:A:266:ILE:O	1:A:268:ARG:N	2.40	0.54
1:A:88:ILE:HG13	1:A:104:LYS:HD3	1.88	0.54
1:A:98:LYS:HG2	1:A:99:LEU:H	1.72	0.54
1:B:99:LEU:C	1:B:101:LYS:H	2.10	0.54
1:B:102:THR:HA	1:B:105:ASP:CB	2.32	0.54
1:A:36:GLY:N	1:A:39:ASP:OD2	2.31	0.54
1:B:244:MSE:HE1	1:B:250:LEU:HG	1.91	0.53
1:B:295:GLU:O	1:B:297:LEU:N	2.42	0.53
1:B:59:VAL:HG22	1:B:64:ILE:HG12	1.91	0.53
1:B:99:LEU:O	1:B:103:GLU:HB2	2.09	0.52
1:A:210:LYS:O	1:B:205:GLY:HA2	2.10	0.52
1:B:14:ARG:HB2	1:B:14:ARG:CZ	2.38	0.52
1:B:100:LYS:O	1:B:104:LYS:HD2	2.10	0.52
1:A:99:LEU:CB	1:A:100:LYS:HB2	2.37	0.52
1:A:108:LYS:O	1:A:111:VAL:HG22	2.08	0.51
1:B:242:PHE:HB3	1:B:253:LEU:HD23	1.92	0.51
1:A:16:ILE:HG13	1:A:18:LEU:HD23	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:HB3	1:A:269:GLU:CG	2.39	0.51
1:B:191:LEU:CD2	1:B:232:LEU:HD21	2.41	0.51
1:B:18:LEU:HD22	1:B:158:LEU:HD22	1.93	0.50
1:B:212:GLN:HG2	1:B:219:ILE:HD11	1.93	0.50
1:A:98:LYS:NZ	1:A:99:LEU:H	2.08	0.50
1:B:20:ALA:O	1:B:21:GLU:HG3	2.10	0.50
1:B:236:TRP:CZ3	1:B:285:GLU:OE2	2.65	0.50
1:A:263:ASN:HB3	1:A:266:ILE:CD1	2.35	0.50
1:A:37:SER:HB2	1:A:117:PRO:HA	1.93	0.50
1:A:77:SER:N	1:A:78:PRO:CD	2.75	0.50
1:B:130:ILE:HG12	1:B:137:ILE:HG12	1.94	0.50
1:A:98:LYS:HG2	1:A:99:LEU:N	2.26	0.50
1:B:90:LYS:C	1:B:92:GLU:H	2.15	0.50
1:A:11:ARG:O	1:A:163:VAL:HA	2.12	0.49
1:A:1:MSE:HE2	1:A:278:ASP:HB3	1.94	0.49
1:B:41:ALA:HA	1:B:71:GLU:O	2.12	0.49
1:A:261:ASP:O	1:A:264:GLU:HB2	2.13	0.49
1:B:134:ASN:N	1:B:134:ASN:ND2	2.60	0.49
1:B:168:MSE:HE1	1:B:294:ILE:HG23	1.95	0.48
1:A:20:ALA:HA	1:A:23:MSE:HB3	1.95	0.48
1:B:265:ASP:HB2	1:B:266:ILE:HD12	1.94	0.48
1:A:279:PHE:CE1	1:A:283:THR:HG21	2.48	0.48
1:B:68:ALA:O	1:B:125:GLN:HA	2.14	0.48
1:B:263:ASN:ND2	1:B:277:ALA:HB1	2.28	0.48
1:A:43:MSE:HE2	1:A:68:ALA:HB1	1.96	0.48
1:B:201:LEU:CD1	1:B:201:LEU:H	2.27	0.48
1:A:242:PHE:HE2	1:A:244:MSE:HE2	1.75	0.48
1:A:99:LEU:CA	1:A:100:LYS:HB2	2.44	0.48
1:B:262:GLN:HG2	1:B:262:GLN:O	2.14	0.47
1:B:239:ARG:NH1	1:B:285:GLU:OE2	2.46	0.47
1:B:168:MSE:HE1	1:B:294:ILE:CA	2.42	0.47
1:A:261:ASP:O	1:A:262:GLN:C	2.53	0.47
1:B:269:GLU:HG2	1:B:269:GLU:O	2.13	0.47
1:A:104:LYS:O	1:A:108:LYS:HB2	2.15	0.47
1:A:8:MSE:CE	1:A:142:ALA:O	2.63	0.47
1:B:268:ARG:HG2	1:B:269:GLU:N	2.30	0.47
1:A:181:ARG:O	1:A:181:ARG:HG2	2.14	0.47
1:A:69:ARG:HD2	1:A:125:GLN:NE2	2.25	0.47
1:A:268:ARG:HB3	1:A:268:ARG:HE	1.52	0.47
1:B:70:LYS:NZ	1:B:72:GLU:OE2	2.48	0.47
1:A:81:LYS:O	1:A:85:GLU:HG3	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:O	1:A:61:ASN:CB	2.58	0.46
1:A:8:MSE:HE2	3:A:312:HOH:O	2.14	0.46
1:B:76:PRO:CB	1:B:78:PRO:HD2	2.45	0.46
1:A:45:TRP:CZ2	1:A:153:LEU:HD13	2.51	0.46
1:A:238:GLN:OE1	1:A:238:GLN:CA	2.63	0.46
1:A:19:ARG:O	1:A:23:MSE:N	2.47	0.46
1:B:236:TRP:HZ3	1:B:285:GLU:OE2	1.98	0.45
1:B:99:LEU:HD12	1:B:103:GLU:OE1	2.16	0.45
1:B:129:TRP:CE3	1:B:138:MSE:CG	2.92	0.45
1:B:2:LEU:CD1	1:B:3:TRP:CD1	2.98	0.45
1:B:266:ILE:HG22	1:B:266:ILE:O	2.16	0.45
1:B:168:MSE:HE3	1:B:299:GLY:N	2.30	0.45
1:B:255:PHE:HB2	1:B:260:ARG:HD3	1.97	0.45
1:B:101:LYS:HG2	1:B:102:THR:H	1.82	0.45
1:B:9:VAL:CG2	1:B:138:MSE:CE	2.94	0.44
1:B:12:LEU:HD11	1:B:16:ILE:HD12	1.99	0.44
1:A:146:LYS:NZ	3:A:310:HOH:O	2.26	0.44
1:B:219:ILE:O	1:B:222:HIS:HB2	2.18	0.44
1:B:95:GLN:O	1:B:96:ALA:CB	2.66	0.44
1:B:217:GLU:O	1:B:221:ASN:HB2	2.18	0.44
1:A:99:LEU:HD22	1:A:100:LYS:HD2	2.00	0.43
1:B:66:ILE:HG21	1:B:66:ILE:HD13	1.64	0.43
1:A:171:PRO:HG2	1:A:174:LEU:HD22	1.99	0.43
1:B:265:ASP:OD1	1:B:266:ILE:N	2.39	0.43
1:A:25:LYS:O	3:A:328:HOH:O	2.21	0.43
1:B:281:LEU:O	1:B:285:GLU:HB2	2.18	0.43
1:A:106:SER:O	1:A:110:GLU:HG3	2.19	0.43
1:B:129:TRP:CE2	1:B:283:THR:HG22	2.54	0.43
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.68	0.43
1:B:77:SER:HA	1:B:80:ILE:HD12	2.00	0.43
1:A:191:LEU:CD2	1:A:232:LEU:HD21	2.49	0.42
1:A:16:ILE:HD12	1:A:18:LEU:HB3	2.01	0.42
1:A:95:GLN:CA	1:A:95:GLN:HE21	2.27	0.42
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.88	0.42
1:B:19:ARG:O	1:B:22:GLU:N	2.51	0.42
1:B:9:VAL:HG13	1:B:138:MSE:CE	2.49	0.42
1:B:176:LEU:HB3	1:B:229:VAL:HB	2.02	0.42
1:B:77:SER:N	1:B:78:PRO:CD	2.83	0.42
1:A:1:MSE:CE	1:A:278:ASP:HB3	2.50	0.41
1:A:49:MSE:HB3	1:A:49:MSE:HE2	1.67	0.41
1:B:76:PRO:C	1:B:78:PRO:HD2	2.41	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ARG:HG2	1:B:269:GLU:H	1.84	0.41
1:A:202:GLU:O	1:A:203:ASP:CB	2.68	0.41
1:B:102:THR:CA	1:B:105:ASP:HB3	2.34	0.41
1:B:199:SER:OG	1:B:204:GLY:HA3	2.19	0.41
1:B:19:ARG:HG3	1:B:22:GLU:OE1	2.19	0.41
1:A:218:GLU:HG2	1:B:222:HIS:CD2	2.56	0.41
1:B:101:LYS:CG	1:B:102:THR:N	2.84	0.41
1:B:194:GLU:HB3	1:B:233:ALA:HB2	2.03	0.41
1:A:129:TRP:CZ2	1:A:283:THR:HB	2.55	0.41
1:A:146:LYS:HG3	1:A:146:LYS:O	2.20	0.41
1:A:16:ILE:O	1:A:18:LEU:N	2.53	0.41
1:A:183:GLY:HA2	1:A:215:THR:CG2	2.48	0.41
1:B:134:ASN:H	1:B:134:ASN:HD22	1.68	0.41
1:B:28:ALA:HA	1:B:56:LEU:HD11	2.03	0.41
1:A:198:LYS:N	1:A:228:VAL:O	2.46	0.40
1:B:131:ASP:C	1:B:131:ASP:OD1	2.58	0.40
1:A:46:VAL:HB	1:A:47:PRO:HD2	2.03	0.40
1:B:103:GLU:O	1:B:107:LEU:HB2	2.21	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	300/303 (99%)	267 (89%)	25 (8%)	8 (3%)	6	6
1	B	299/303 (99%)	257 (86%)	27 (9%)	15 (5%)	2	1
All	All	599/606 (99%)	524 (88%)	52 (9%)	23 (4%)	4	3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ALA
1	A	100	LYS
1	B	37	SER
1	B	96	ALA
1	B	98	LYS
1	A	99	LEU
1	A	267	ASP
1	B	15	GLU
1	B	24	GLU
1	B	40	MSE
1	B	89	ALA
1	B	133	VAL
1	B	262	GLN
1	A	15	GLU
1	A	17	SER
1	B	21	GLU
1	B	301	ALA
1	A	101	LYS
1	B	17	SER
1	B	296	GLY
1	A	61	ASN
1	B	20	ALA
1	B	95	GLN

### 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	258/246 (105%)	236 (92%)	22 (8%)	12	19
1	B	257/246 (104%)	216 (84%)	41 (16%)	3	3
All	All	515/492 (105%)	452 (88%)	63 (12%)	6	7

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

Mol	Chain	Res	Type
1	A	19	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	22	GLU
1	A	30	MSE
1	A	54	ASP
1	A	66	ILE
1	A	82	GLN
1	A	87	LYS
1	A	88	ILE
1	A	94	GLU
1	A	95	GLN
1	A	97	ARG
1	A	98	LYS
1	A	109	ASP
1	A	116	LEU
1	A	124	SER
1	A	146	LYS
1	A	153	LEU
1	A	173	GLU
1	A	202	GLU
1	A	238	GLN
1	A	268	ARG
1	A	269	GLU
1	B	2	LEU
1	B	8	MSE
1	B	12	LEU
1	B	15	GLU
1	B	16	ILE
1	B	19	ARG
1	B	21	GLU
1	B	25	LYS
1	B	29	SER
1	B	42	LYS
1	B	49	MSE
1	B	54	ASP
1	B	84	LEU
1	B	90	LYS
1	B	94	GLU
1	B	98	LYS
1	B	103	GLU
1	B	104	LYS
1	B	105	ASP
1	B	107	LEU
1	B	122	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	134	ASN
1	B	138	MSE
1	B	146	LYS
1	B	157	SER
1	B	160	SER
1	B	164	VAL
1	B	168	MSE
1	B	176	LEU
1	B	184	SER
1	B	187	GLN
1	B	197	LEU
1	B	201	LEU
1	B	202	GLU
1	B	220	THR
1	B	221	ASN
1	B	257	ASP
1	B	268	ARG
1	B	269	GLU
1	B	274	ARG
1	B	276	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	63	GLN
1	A	95	GLN
1	A	125	GLN
1	A	222	HIS
1	A	292	ASN
1	B	58	HIS
1	B	82	GLN
1	B	134	ASN
1	B	187	GLN
1	B	222	HIS
1	B	263	ASN
1	B	291	GLN
1	B	292	ASN
1	B	302	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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	289/303 (95%)	0.20	23 (7%) 13 12	16, 41, 107, 127	0
1	B	289/303 (95%)	0.21	25 (8%) 11 10	28, 47, 101, 118	0
All	All	578/606 (95%)	0.21	48 (8%) 12 11	16, 45, 106, 127	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	266	ILE	5.5
1	B	93	ALA	5.4
1	A	101	LYS	5.3
1	A	267	ASP	4.8
1	A	96	ALA	4.4
1	A	102	THR	4.3
1	A	95	GLN	4.1
1	A	98	LYS	4.0
1	B	99	LEU	3.8
1	A	302	GLN	3.7
1	B	202	GLU	3.6
1	B	92	GLU	3.6
1	A	17	SER	3.4
1	B	91	LEU	3.4
1	B	98	LYS	3.3
1	A	89	ALA	3.3
1	A	268	ARG	3.3
1	B	22	GLU	3.2
1	A	99	LEU	3.2
1	B	301	ALA	3.2
1	B	101	LYS	3.1
1	B	94	GLU	3.1
1	A	93	ALA	3.0
1	B	89	ALA	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	97	ARG	2.7
1	B	106	SER	2.7
1	A	265	ASP	2.7
1	B	17	SER	2.6
1	B	265	ASP	2.6
1	B	271	PHE	2.6
1	A	14	ARG	2.6
1	B	105	ASP	2.5
1	B	109	ASP	2.5
1	B	18	LEU	2.5
1	A	105	ASP	2.5
1	B	268	ARG	2.5
1	A	106	SER	2.4
1	B	14	ARG	2.4
1	B	97	ARG	2.4
1	A	18	LEU	2.4
1	B	219	ILE	2.4
1	B	19	ARG	2.2
1	A	92	GLU	2.2
1	A	137	ILE	2.1
1	A	94	GLU	2.1
1	A	271	PHE	2.1
1	B	61	ASN	2.1
1	A	88	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	304	1/1	0.96	0.14	-	59,59,59,59	0
2	CA	B	304	1/1	0.94	0.11	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.