

Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2021 – 08:48 AM EDT

:	1Z6R
:	Crystal structure of Mlc from Escherichia coli
:	Schiefner, A.; Gerber, K.; Seitz, S.; Welte, W.; Diederichs, K.; Boos, W.
:	2005-03-23
:	2.70 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* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) 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	:	2.23.2
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)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 2.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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 chai	n	
1	А	406	64%	24%	6% 6%
1	В	406	4% 60%	29%	5% 6%
1	С	406	56%	33%	• • 6%
1	D	406	61%	30%	• 6%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11728 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.

Mol	Chain	Residues		Atoms					ZeroOcc	AltConf	Trace
1	Λ	380	Total	С	Ν	0	S	Se	0	0	0
1	Л	362	2931	1855	514	549	4	9	0		U
1	В	382	Total	С	Ν	Ο	S	Se	0	0	0
1			2931	1855	514	549	4	9	0	0	0
1	1 C	380	Total	С	Ν	0	S	Se	0	0	0
1		302	2931	1855	514	549	4	9	0	0	U
1	1 D	380	Total	С	Ν	0	S	Se	0	0	0
	362	2931	1855	514	549	4	9	0	0	U	

• Molecule 1 is a protein called Mlc protein.

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	MSE	MET	modified residue	UNP P50456
А	52	HIS	ARG	engineered mutation	UNP P50456
А	54	MSE	MET	modified residue	UNP P50456
А	167	MSE	MET	modified residue	UNP P50456
А	176	MSE	MET	modified residue	UNP P50456
А	201	MSE	MET	modified residue	UNP P50456
А	286	MSE	MET	modified residue	UNP P50456
А	289	MSE	MET	modified residue	UNP P50456
А	329	MSE	MET	modified residue	UNP P50456
A	384	MSE	MET	modified residue	UNP P50456
А	394	MSE	MET	modified residue	UNP P50456
В	1	MSE	MET	modified residue	UNP P50456
В	52	HIS	ARG	engineered mutation	UNP P50456
В	54	MSE	MET	modified residue	UNP P50456
В	167	MSE	MET	modified residue	UNP P50456
В	176	MSE	MET	modified residue	UNP P50456
В	201	MSE	MET	modified residue	UNP P50456
В	286	MSE	MET	modified residue	UNP P50456
В	289	MSE	MET	modified residue	UNP P50456
В	329	MSE	MET	modified residue	UNP P50456
В	384	MSE	MET	modified residue	UNP P50456



Chain	Residue	Modelled	Actual	Comment	Reference
В	394	MSE	MET	modified residue	UNP P50456
С	1	MSE	MET	modified residue	UNP P50456
С	52	HIS	ARG	engineered mutation	UNP P50456
С	54	MSE	MET	modified residue	UNP P50456
С	167	MSE	MET	modified residue	UNP P50456
С	176	MSE	MET	modified residue	UNP P50456
С	201	MSE	MET	modified residue	UNP P50456
С	286	MSE	MET	modified residue	UNP P50456
С	289	MSE	MET	modified residue	UNP P50456
С	329	MSE	MET	modified residue	UNP P50456
С	384	MSE	MET	modified residue	UNP P50456
С	394	MSE	MET	modified residue	UNP P50456
D	1	MSE	MET	modified residue	UNP P50456
D	52	HIS	ARG	engineered mutation	UNP P50456
D	54	MSE	MET	modified residue	UNP P50456
D	167	MSE	MET	modified residue	UNP P50456
D	176	MSE	MET	modified residue	UNP P50456
D	201	MSE	MET	modified residue	UNP P50456
D	286	MSE	MET	modified residue	UNP P50456
D	289	MSE	MET	modified residue	UNP P50456
D	329	MSE	MET	modified residue	UNP P50456
D	384	MSE	MET	modified residue	UNP P50456
D	394	MSE	MET	modified residue	UNP P50456

• Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	Total Zn 1 1	0	0
2	В	1	Total Zn 1 1	0	0
2	С	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0





3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Mlc protein



• Molecule 1: Mlc protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	235.95Å 74.71Å 154.95Å	Deperitor
a, b, c, α , β , γ	90.00° 129.15° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\hat{\mathbf{A}})$	19.94 - 2.70	Depositor
Resolution (A)	19.94 - 2.70	EDS
% Data completeness	100.0 (19.94-2.70)	Depositor
(in resolution range)	99.0(19.94-2.70)	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	0.10	Depositor
$< I/\sigma(I) > 1$	$1.37 (at 2.71 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D.	0.203 , 0.263	Depositor
II, II, <i>free</i>	0.201 , 0.258	DCC
R_{free} test set	2856 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	67.0	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.33 , 80.8	EDS
L-test for $twinning^2$	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.025 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11728	wwPDB-VP
Average B, all atoms $(Å^2)$	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

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: ZN

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	Bo	ond lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.66	5/2969~(0.2%)	0.75	3/4010~(0.1%)	
1	В	0.78	1/2969~(0.0%)	0.81	3/4010~(0.1%)	
1	С	1.00	10/2969~(0.3%)	0.83	9/4010~(0.2%)	
1	D	0.78	12/2969~(0.4%)	0.73	4/4010~(0.1%)	
All	All	0.82	28/11876~(0.2%)	0.78	19/16040~(0.1%)	

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	С	0	3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	285	SER	CB-OG	26.01	1.76	1.42
1	С	38	ARG	CZ-NH1	22.97	1.62	1.33
1	В	406	GLY	C-O	16.27	1.49	1.23
1	С	77	GLY	N-CA	13.24	1.66	1.46
1	D	133	ASP	CG-OD1	12.36	1.53	1.25
1	D	130	SER	CB-OG	10.45	1.55	1.42
1	А	138	ARG	CZ-NH1	9.77	1.45	1.33
1	С	38	ARG	CG-CD	9.75	1.76	1.51
1	D	139	HIS	CE1-NE2	9.56	1.54	1.32
1	D	406	GLY	C-O	9.31	1.38	1.23
1	D	126	ASP	CG-OD2	8.46	1.44	1.25
1	D	260	GLY	C-O	8.07	1.36	1.23
1	A	77	GLY	N-CA	8.02	1.58	1.46
1	D	126	ASP	CG-OD1	7.68	1.43	1.25



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
1	С	286	MSE	C-O	-7.04	1.09	1.23
1	С	44	PRO	C-N	6.94	1.50	1.34
1	С	283	ASN	CG-OD1	6.89	1.39	1.24
1	D	139	HIS	CG-ND1	6.75	1.53	1.38
1	С	41	GLN	C-O	-6.30	1.11	1.23
1	А	138	ARG	CZ-NH2	6.17	1.41	1.33
1	А	306	ARG	CZ-NH1	6.14	1.41	1.33
1	С	306	ARG	CZ-NH1	5.51	1.40	1.33
1	D	378	PHE	CE1-CZ	5.50	1.47	1.37
1	С	286	MSE	C-N	5.49	1.46	1.34
1	D	260	GLY	C-N	5.39	1.46	1.34
1	D	378	PHE	CG-CD2	5.25	1.46	1.38
1	А	138	ARG	CD-NE	5.08	1.55	1.46
1	D	133	ASP	C-O	5.03	1.32	1.23

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All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	С	38	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	С	33	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	А	138	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	С	44	PRO	O-C-N	7.72	135.05	122.70
1	В	406	GLY	CA-C-O	-6.51	108.88	120.60
1	С	306	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	126	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	А	364	LEU	CA-CB-CG	6.00	129.11	115.30
1	С	282	LEU	CA-CB-CG	5.69	128.38	115.30
1	D	210	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	В	42	LEU	CA-CB-CG	5.54	128.05	115.30
1	С	44	PRO	CA-C-N	-5.34	105.44	117.20
1	В	103	ASP	CB-CA-C	-5.29	99.82	110.40
1	С	286	MSE	CA-C-N	-5.24	105.68	117.20
1	С	324	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	С	78	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	А	306	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	D	364	LEU	CA-CB-CG	5.04	126.89	115.30
1	D	260	GLY	CA-C-O	5.01	129.62	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	С	286	MSE	Mainchain
1	С	38	ARG	Sidechain
1	С	44	PRO	Mainchain

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	А	2931	0	2988	70	0
1	В	2931	0	2988	92	0
1	С	2931	0	2988	88	0
1	D	2931	0	2988	70	0
2	А	1	0	0	0	0
2	В	1	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
All	All	11728	0	11952	307	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 13.

All (307) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:38:ARG:CG	1:C:38:ARG:CD	1.76	1.57
1:B:384:MSE:CE	1:B:384:MSE:SE	2.16	1.44
1:D:289:MSE:SE	1:D:289:MSE:CE	2.15	1.43
1:C:285:SER:OG	1:C:285:SER:CB	1.76	1.33
1:D:91:ARG:CZ	1:D:380:ASN:HD21	1.59	1.13
1:B:164:VAL:HG11	1:B:167:MSE:HE2	1.26	1.13
1:C:164:VAL:HG11	1:C:167:MSE:HE2	1.34	1.09
1:D:91:ARG:NH2	1:D:380:ASN:HD21	1.52	1.07
1:B:13:ILE:HD12	1:B:13:ILE:H	1.26	1.01
1:A:148:SER:HA	1:A:188:VAL:HG13	1.43	0.97
1:C:132:ILE:HD13	1:C:182:LEU:HD21	1.50	0.93
1:B:176:MSE:HE3	1:B:178:LEU:HG	1.52	0.91
1:A:264:CYS:O	1:A:267:THR:HB	1.70	0.90



	io ao pagoni	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:176:MSE:HE3	1:C:178:LEU:HG	1.55	0.88
1:B:54:MSE:HE3	1:B:60:VAL:HG21	1.55	0.88
1:C:178:LEU:HD22	1:C:182:LEU:HD12	1.55	0.87
1:C:148:SER:HA	1:C:188:VAL:HG13	1.57	0.85
1:B:376:THR:CG2	1:B:378:PHE:O	2.25	0.84
1:B:148:SER:HA	1:B:188:VAL:HG13	1.59	0.84
1:D:91:ARG:CZ	1:D:380:ASN:ND2	2.41	0.83
1:A:402:ARG:O	1:A:405:GLN:HB2	1.79	0.82
1:A:164:VAL:HG11	1:A:167:MSE:HE2	1.58	0.82
1:B:245:ILE:O	1:B:248:THR:HG23	1.80	0.81
1:D:218:VAL:HG21	1:D:326:LEU:HD11	1.60	0.81
1:B:132:ILE:HD12	1:B:182:LEU:HD21	1.64	0.80
1:C:164:VAL:HG11	1:C:167:MSE:CE	2.11	0.79
1:D:91:ARG:NH2	1:D:380:ASN:ND2	2.30	0.79
1:C:264:CYS:O	1:C:267:THR:HB	1.83	0.78
1:C:38:ARG:CD	1:C:38:ARG:CB	2.60	0.77
1:C:89:SER:OG	1:C:383:THR:HB	1.84	0.77
1:C:216:ILE:HD12	1:C:335:PRO:HG3	1.67	0.77
1:B:194:HIS:HD2	1:B:196:ILE:H	1.33	0.77
1:C:194:HIS:HD2	1:C:196:ILE:H	1.33	0.76
1:A:183:GLU:HG3	1:A:190:VAL:HG23	1.69	0.74
1:D:148:SER:HA	1:D:188:VAL:HG13	1.70	0.74
1:D:167:MSE:HG2	1:D:173:VAL:HG21	1.69	0.74
1:B:178:LEU:HD22	1:B:182:LEU:CD1	2.18	0.73
1:C:343:PRO:O	1:C:346:LYS:HG2	1.87	0.73
1:B:166:ARG:HG3	1:B:166:ARG:HH11	1.54	0.72
1:A:51:VAL:HA	1:A:54:MSE:HE2	1.70	0.72
1:D:167:MSE:HE3	1:D:173:VAL:HG11	1.71	0.72
1:B:194:HIS:CD2	1:B:196:ILE:H	2.09	0.71
1:A:54:MSE:HE3	1:A:60:VAL:HG21	1.72	0.71
1:A:277:LEU:CD2	1:D:286:MSE:HE2	2.20	0.71
1:A:206:PHE:HZ	1:A:391:LYS:HG3	1.55	0.71
1:B:84:ALA:HA	1:B:144:GLU:HG2	1.73	0.70
1:D:176:MSE:HE3	1:D:178:LEU:HG	1.72	0.70
1:B:117:ALA:O	1:B:127:ARG:NH2	2.24	0.70
1:A:216:ILE:HD12	1:A:335:PRO:HG3	1.73	0.69
1:C:214:ASP:HA	1:C:229:ILE:O	1.91	0.69
1:D:218:VAL:CG2	1:D:326:LEU:HD11	2.22	0.69
1:B:221:ASP:HB3	1:B:223:ASN:H	1.57	0.69
1:D:200:THR:HA	1:D:217:GLN:OE1	1.93	0.69
1:A:148:SER:HA	1:A:188:VAL:CG1	2.22	0.67



	A state of the sta	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:130:SER:O	1:B:134:GLN:HG3	1.94	0.67
1:C:155:GLY:O	1:C:157:ILE:HD12	1.95	0.67
1:D:139:HIS:HB3	1:D:142:LYS:HD2	1.76	0.66
1:B:13:ILE:H	1:B:13:ILE:CD1	1.99	0.66
1:B:86:HIS:CD2	1:B:144:GLU:H	2.14	0.66
1:B:178:LEU:HD22	1:B:182:LEU:HD12	1.76	0.66
1:B:132:ILE:CD1	1:B:182:LEU:HD21	2.26	0.65
1:B:264:CYS:O	1:B:267:THR:HB	1.95	0.65
1:B:199:TRP:HZ2	1:B:376:THR:HG21	1.62	0.65
1:D:164:VAL:HG11	1:D:167:MSE:HE2	1.78	0.65
1:B:143:LEU:HD22	1:B:144:GLU:O	1.97	0.65
1:A:280:LEU:HD22	1:D:292:GLY:HA2	1.79	0.64
1:C:167:MSE:HE3	1:C:173:VAL:HG11	1.79	0.64
1:B:80:VAL:HG12	1:B:82:THR:HG23	1.79	0.64
1:C:105:SER:O	1:C:106:SER:HB3	1.97	0.63
1:C:12:GLN:HG3	1:C:13:ILE:HD12	1.81	0.63
1:C:183:GLU:HG2	1:C:188:VAL:O	1.99	0.63
1:B:376:THR:HG23	1:B:378:PHE:O	1.97	0.63
1:C:255:LYS:HD2	1:C:267:THR:HG23	1.82	0.62
1:C:117:ALA:O	1:C:127:ARG:NH2	2.32	0.62
1:B:244:GLU:HG3	1:B:247:HIS:HD2	1.64	0.62
1:C:51:VAL:HA	1:C:54:MSE:CE	2.31	0.61
1:C:89:SER:HG	1:C:383:THR:HB	1.65	0.61
1:D:341:GLY:HA2	1:D:376:THR:HG21	1.82	0.61
1:D:341:GLY:HA2	1:D:376:THR:CG2	2.30	0.61
1:B:90:LEU:HD21	1:B:132:ILE:HD11	1.83	0.61
1:C:199:TRP:HZ2	1:C:376:THR:HG21	1.66	0.61
1:A:82:THR:HG22	1:A:104:LEU:HB2	1.83	0.61
1:A:297:VAL:HG11	1:A:343:PRO:HB2	1.81	0.61
1:A:176:MSE:HE3	1:A:178:LEU:HG	1.82	0.61
1:A:331:ASN:HD22	1:B:248:THR:HG22	1.65	0.61
1:A:183:GLU:HG3	1:A:190:VAL:CG2	2.33	0.59
1:C:23:ARG:HA	1:C:395:TYR:CE2	2.37	0.59
1:B:80:VAL:CG1	1:B:82:THR:HG23	2.33	0.59
1:C:279:GLN:O	1:C:283:ASN:ND2	2.36	0.59
1:D:224:VAL:HG11	1:D:265:LEU:HD13	1.85	0.59
1:B:149:ILE:HD11	1:B:186:THR:HG21	1.85	0.59
1:C:152:THR:HG23	1:C:195:ASP:HA	1.84	0.58
1:C:149:ILE:HD11	1:C:186:THR:HG21	1.85	0.58
1:D:90:LEU:HD21	1:D:132:ILE:HD11	1.86	0.58
1:B:287:SER:HB3	1:C:254:GLY:HA2	1.83	0.58



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:267:THR:HG22	1:B:268:ILE:HD12	1.86	0.58
1:B:217:GLN:O	1:B:226:ALA:HA	2.04	0.58
1:A:164:VAL:HG11	1:A:167:MSE:CE	2.33	0.57
1:C:149:ILE:HB	1:C:190:VAL:HG22	1.86	0.57
1:C:60:VAL:HG12	1:C:78:LEU:HD12	1.87	0.57
1:C:103:ASP:HB3	1:C:105:SER:H	1.70	0.57
1:A:33:ARG:HG2	1:A:47:ILE:HG23	1.86	0.57
1:D:196:ILE:HD13	1:D:225:GLY:HA3	1.87	0.56
1:B:183:GLU:HG3	1:B:190:VAL:HG23	1.87	0.56
1:A:332:LEU:HD21	1:B:329:MSE:HE3	1.88	0.56
1:A:394:MSE:SE	1:A:399:LEU:HD13	2.56	0.56
1:A:212:ALA:HA	1:A:336:GLN:HE22	1.71	0.56
1:B:25:ILE:HG22	1:B:80:VAL:HG23	1.88	0.56
1:B:25:ILE:HD12	1:B:54:MSE:CE	2.36	0.55
1:B:271:VAL:HA	1:B:274:ILE:HD12	1.88	0.55
1:D:217:GLN:O	1:D:226:ALA:HA	2.06	0.55
1:C:51:VAL:HA	1:C:54:MSE:HE3	1.89	0.55
1:B:103:ASP:HB3	1:B:105:SER:H	1.72	0.54
1:B:61:GLN:OE1	1:B:81:GLU:HG2	2.08	0.54
1:C:84:ALA:HA	1:C:144:GLU:HG2	1.90	0.54
1:D:25:ILE:HG22	1:D:80:VAL:HG23	1.90	0.54
1:B:270:SER:O	1:B:274:ILE:HG13	2.09	0.53
1:D:213:ARG:HH11	1:D:213:ARG:HB3	1.72	0.53
1:B:101:LEU:HB3	1:B:109:VAL:HB	1.91	0.53
1:C:29:GLY:HA2	1:C:30:PRO:C	2.29	0.53
1:C:394:MSE:SE	1:C:399:LEU:HD13	2.58	0.53
1:B:290:LEU:HD21	1:B:300:LEU:HA	1.91	0.53
1:D:109:VAL:HG12	1:D:110:VAL:HG22	1.91	0.53
1:A:206:PHE:CZ	1:A:391:LYS:HG3	2.39	0.52
1:B:199:TRP:CZ2	1:B:376:THR:HG21	2.42	0.52
1:A:216:ILE:CD1	1:A:335:PRO:HG3	2.37	0.52
1:D:189:PRO:HG2	1:D:399:LEU:HD23	1.91	0.52
1:C:331:ASN:HD21	1:C:363:ALA:HA	1.75	0.52
1:D:123:PRO:HD2	1:D:126:ASP:OD2	2.09	0.52
1:A:92:ILE:HD12	1:A:153:LEU:HD23	1.91	0.52
1:D:151:ILE:HB	1:D:192:ILE:HG12	1.91	0.52
1:D:340:ILE:HD13	1:D:373:VAL:HG13	1.92	0.52
1:B:376:THR:HG21	1:B:378:PHE:O	2.05	0.51
1:B:381:GLN:H	1:B:384:MSE:HE3	1.75	0.51
1:C:120:ASP:CG	1:C:121:ASP:N	2.64	0.51
1:C:285:SER:OG	1:C:285:SER:CA	2.55	0.51



	lo uo page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:54:MSE:HG3	1:D:404:LEU:HD21	1.91	0.51
1:B:236:HIS:O	1:B:237:ALA:C	2.49	0.51
1:A:376:THR:HG23	1:A:378:PHE:O	2.09	0.51
1:B:136:PHE:O	1:B:140:GLN:HB2	2.11	0.51
1:C:394:MSE:HE3	1:C:400:LEU:HG	1.93	0.51
1:A:224:VAL:HG11	1:A:265:LEU:HD13	1.92	0.51
1:D:209:SER:HB2	1:D:215:VAL:HG21	1.93	0.51
1:D:148:SER:HA	1:D:188:VAL:CG1	2.39	0.51
1:A:147:THR:O	1:A:189:PRO:HD2	2.11	0.51
1:C:208:ALA:HB2	1:C:377:GLN:HB2	1.92	0.50
1:D:53:GLU:HB3	1:D:404:LEU:HD22	1.94	0.50
1:D:199:TRP:HD1	1:D:199:TRP:O	1.94	0.50
1:D:213:ARG:NH1	1:D:231:ASP:HA	2.26	0.50
1:B:384:MSE:CE	1:B:384:MSE:CG	2.89	0.50
1:D:57:ALA:O	1:D:85:TRP:HZ2	1.94	0.50
1:D:328:ILE:O	1:D:332:LEU:HG	2.10	0.50
1:B:91:ARG:HG3	1:B:152:THR:HG22	1.94	0.50
1:C:120:ASP:CG	1:C:121:ASP:H	2.15	0.50
1:D:208:ALA:HB2	1:D:377:GLN:HB2	1.94	0.50
1:A:151:ILE:HB	1:A:192:ILE:HG12	1.93	0.50
1:A:278:ALA:O	1:A:282:LEU:HB2	2.12	0.50
1:A:251:ASP:O	1:A:263:GLY:HA3	2.12	0.50
1:B:25:ILE:HD12	1:B:54:MSE:HE1	1.93	0.50
1:D:247:HIS:HA	1:D:264:CYS:HB3	1.94	0.49
1:A:282:LEU:HD11	1:A:290:LEU:CB	2.43	0.49
1:B:286:MSE:HE1	1:C:318:VAL:HG22	1.93	0.49
1:C:55:LEU:HD21	1:C:78:LEU:HD11	1.95	0.49
1:B:339:LEU:HD23	1:B:374:GLU:HG3	1.94	0.49
1:D:22:TYR:CZ	1:D:394:MSE:HE2	2.48	0.49
1:D:201:MSE:HE3	1:D:234:LEU:HB2	1.95	0.49
1:B:159:THR:HG21	1:B:193:GLN:NE2	2.28	0.48
1:C:352:PHE:CD2	1:C:352:PHE:N	2.80	0.48
1:A:213:ARG:HB3	1:A:213:ARG:HH11	1.78	0.48
1:A:245:ILE:HD13	1:A:245:ILE:HG21	1.54	0.48
1:A:277:LEU:HD21	1:D:286:MSE:HE2	1.95	0.48
1:B:59:LEU:HD21	1:B:403:LEU:HD13	1.95	0.48
1:A:282:LEU:HD23	1:A:291:HIS:NE2	2.29	0.48
1:B:214:ASP:HA	1:B:229:ILE:O	2.13	0.48
1:D:251:ASP:HA	1:D:252:PRO:HD2	1.73	0.48
1:A:86:HIS:CD2	1:A:144:GLU:H	2.32	0.48
1:A:194:HIS:HD2	1:A:196:ILE:H	1.61	0.48



	lo uo pugom	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:87:TYR:OH	1:A:387:ALA:HA	2.13	0.48
1:A:92:ILE:HB	1:A:153:LEU:HB3	1.96	0.48
1:C:309:LEU:O	1:C:313:ASP:HB3	2.14	0.48
1:B:343:PRO:O	1:B:346:LYS:HG2	2.14	0.47
1:B:251:ASP:O	1:B:263:GLY:HA3	2.13	0.47
1:A:282:LEU:HD11	1:A:290:LEU:HB3	1.96	0.47
1:D:167:MSE:HG2	1:D:173:VAL:CG2	2.40	0.47
1:C:51:VAL:HA	1:C:54:MSE:HE2	1.95	0.47
1:C:79:VAL:HG22	1:C:80:VAL:H	1.80	0.47
1:D:22:TYR:HB2	1:D:400:LEU:HD11	1.96	0.47
1:A:80:VAL:CG1	1:A:82:THR:HG23	2.45	0.47
1:D:201:MSE:HE3	1:D:234:LEU:HD13	1.96	0.47
1:D:371:ILE:O	1:D:371:ILE:HG23	2.14	0.47
1:C:245:ILE:HG22	1:D:332:LEU:HD21	1.96	0.47
1:D:194:HIS:NE2	1:D:196:ILE:HD12	2.30	0.47
1:B:154:PRO:HB2	1:B:168:PRO:HG2	1.97	0.47
1:D:252:PRO:HB2	1:D:253:TYR:CD1	2.49	0.47
1:A:54:MSE:HB3	1:A:60:VAL:HB	1.96	0.47
1:B:166:ARG:HH11	1:B:166:ARG:CG	2.23	0.47
1:B:218:VAL:HG21	1:B:326:LEU:HD22	1.97	0.46
1:B:245:ILE:O	1:B:248:THR:CG2	2.59	0.46
1:B:255:LYS:CG	1:B:267:THR:HG23	2.45	0.46
1:A:255:LYS:HG3	1:A:267:THR:HG23	1.97	0.46
1:C:87:TYR:HE2	1:C:103:ASP:O	1.99	0.46
1:C:21:VAL:O	1:C:25:ILE:HG13	2.15	0.46
1:A:117:ALA:O	1:A:127:ARG:NH2	2.49	0.46
1:A:288:SER:OG	1:A:290:LEU:HD12	2.15	0.46
1:A:289:MSE:HE2	1:A:289:MSE:HB3	1.89	0.46
1:C:33:ARG:HG2	1:C:47:ILE:CG2	2.46	0.46
1:C:207:GLY:HA2	1:C:378:PHE:HE1	1.80	0.46
1:A:244:GLU:HG3	1:A:247:HIS:HD2	1.81	0.46
1:B:115:GLU:OE2	1:B:115:GLU:HA	2.16	0.46
1:A:87:TYR:CG	1:A:390:VAL:HG21	2.51	0.45
1:C:244:GLU:HG2	1:D:364:LEU:HD12	1.98	0.45
1:B:15:GLN:HA	1:B:401:ILE:HD13	1.98	0.45
1:C:178:LEU:HD22	1:C:182:LEU:CD1	2.36	0.45
1:C:399:LEU:HD22	1:C:403:LEU:HG	1.99	0.45
1:D:193:GLN:HB2	1:D:389:LEU:HD11	1.98	0.45
1:D:278:ALA:HB3	1:D:295:LEU:HD11	1.97	0.45
1:C:13:ILE:HD13	1:D:39:LEU:O	2.16	0.45
1:A:322:VAL:HG12	1:A:326:LEU:HD22	1.97	0.45



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:235:LEU:O	1:A:236:HIS:HB2	2.16	0.45
1:A:212:ALA:HA	1:A:336:GLN:NE2	2.30	0.45
1:C:105:SER:O	1:C:106:SER:CB	2.63	0.45
1:B:92:ILE:O	1:B:154:PRO:HD3	2.17	0.45
1:B:147:THR:O	1:B:148:SER:HB3	2.16	0.45
1:C:251:ASP:O	1:C:263:GLY:HA3	2.16	0.45
1:A:91:ARG:HD2	1:A:382:GLY:O	2.17	0.44
1:B:126:ASP:O	1:B:127:ARG:C	2.55	0.44
1:C:352:PHE:N	1:C:352:PHE:HD2	2.14	0.44
1:C:365:PRO:HG2	1:D:259:CYS:O	2.18	0.44
1:B:365:PRO:O	1:B:369:GLN:HB2	2.17	0.44
1:C:157:ILE:O	1:C:240:SER:HB2	2.17	0.44
1:A:42:LEU:HD23	1:A:46:SER:HB3	1.99	0.44
1:B:33:ARG:HG2	1:B:47:ILE:HG22	2.00	0.44
1:D:245:ILE:HG13	1:D:246:GLY:N	2.33	0.44
1:B:182:LEU:HB3	1:B:190:VAL:HG21	1.99	0.44
1:B:304:ALA:CB	1:B:315:ILE:HD12	2.48	0.44
1:C:181:ALA:O	1:C:185:HIS:HB2	2.18	0.44
1:A:200:THR:HA	1:A:217:GLN:OE1	2.18	0.44
1:C:305:LEU:HD23	1:C:350:ILE:HD12	1.99	0.44
1:B:155:GLY:C	1:B:157:ILE:HD12	2.38	0.43
1:B:384:MSE:HG3	1:B:385:ALA:N	2.32	0.43
1:C:305:LEU:HD21	1:C:347:ALA:HA	1.99	0.43
1:A:259:CYS:O	1:B:365:PRO:HG2	2.17	0.43
1:C:322:VAL:HG12	1:C:326:LEU:HD22	2.01	0.43
1:A:147:THR:HG22	1:A:403:LEU:HD21	1.99	0.43
1:A:234:LEU:HA	1:A:234:LEU:HD12	1.69	0.43
1:A:63:LEU:HD12	1:A:79:VAL:HG21	1.99	0.43
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.70	0.43
1:A:214:ASP:OD1	1:A:230:THR:HG22	2.19	0.43
1:B:148:SER:HA	1:B:188:VAL:CG1	2.40	0.43
1:D:217:GLN:HG3	1:D:339:LEU:HB2	2.00	0.43
1:C:14:LYS:HB2	1:D:41:GLN:HE22	1.82	0.43
1:C:87:TYR:CE2	1:C:103:ASP:O	2.72	0.43
1:C:218:VAL:HG13	1:C:245:ILE:HD11	2.00	0.43
1:C:22:TYR:HB2	1:C:400:LEU:HD11	2.01	0.43
1:D:80:VAL:HG12	1:D:82:THR:HG23	2.01	0.43
1:A:22:TYR:HB2	1:A:400:LEU:HD11	2.01	0.43
1:A:151:ILE:HD11	1:A:182:LEU:CD1	2.49	0.43
1:D:86:HIS:HA	1:D:102:ARG:O	2.19	0.43
1:C:87:TYR:CG	1:C:390:VAL:HG21	2.54	0.42



	le as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:82:THR:HG22	1:A:104:LEU:CB	2.48	0.42
1:C:91:ARG:HA	1:C:152:THR:O	2.18	0.42
1:B:160:GLU:OE1	1:B:238:GLY:O	2.38	0.42
1:C:148:SER:HA	1:C:188:VAL:CG1	2.38	0.42
1:C:221:ASP:C	1:C:223:ASN:H	2.21	0.42
1:C:224:VAL:HG11	1:C:265:LEU:HD13	2.00	0.42
1:C:17:ASN:OD1	1:C:42:LEU:HD11	2.20	0.42
1:C:15:GLN:HA	1:C:401:ILE:HD13	2.02	0.42
1:B:369:GLN:HG3	1:B:370:HIS:ND1	2.34	0.42
1:C:26:ASP:OD2	1:C:395:TYR:OH	2.33	0.42
1:C:218:VAL:HG21	1:C:326:LEU:HD21	2.01	0.42
1:B:90:LEU:HD21	1:B:132:ILE:CD1	2.49	0.42
1:B:152:THR:HG23	1:B:195:ASP:HA	2.02	0.42
1:C:290:LEU:HD11	1:C:311:ALA:HB2	2.01	0.42
1:D:37:SER:HA	1:D:47:ILE:HD13	2.02	0.42
1:A:90:LEU:HD12	1:A:99:LEU:HA	2.01	0.41
1:B:178:LEU:CD2	1:B:182:LEU:CD1	2.95	0.41
1:D:173:VAL:O	1:D:173:VAL:HG23	2.19	0.41
1:B:193:GLN:HG3	1:B:197:SER:OG	2.19	0.41
1:B:29:GLY:HA2	1:B:30:PRO:C	2.41	0.41
1:B:153:LEU:CD1	1:B:157:ILE:HG12	2.50	0.41
1:B:396:ASN:C	1:B:396:ASN:OD1	2.59	0.41
1:C:17:ASN:O	1:C:21:VAL:HG23	2.21	0.41
1:B:25:ILE:HD12	1:B:54:MSE:HE3	2.02	0.41
1:B:266:GLU:O	1:B:270:SER:HB3	2.21	0.41
1:D:219:VAL:O	1:D:224:VAL:HA	2.20	0.41
1:A:255:LYS:HE2	1:A:267:THR:HG23	2.03	0.41
1:C:194:HIS:CD2	1:C:196:ILE:H	2.24	0.41
1:D:191:TYR:OH	1:D:399:LEU:HG	2.20	0.41
1:D:218:VAL:HG21	1:D:326:LEU:CD1	2.42	0.41
1:B:153:LEU:HD13	1:B:157:ILE:HD11	2.02	0.41
1:B:255:LYS:HG3	1:B:267:THR:HG23	2.03	0.41
1:C:116:LEU:HD13	1:C:124:LEU:HD11	2.03	0.41
1:C:196:ILE:HD12	1:C:225:GLY:HA3	2.03	0.41
1:C:383:THR:O	1:C:385:ALA:N	2.54	0.41
1:D:199:TRP:O	1:D:199:TRP:CD1	2.72	0.41
1:A:343:PRO:O	1:A:346:LYS:HG2	2.21	0.41
1:C:326:LEU:HD12	1:C:326:LEU:HA	1.83	0.41
1:D:48:THR:O	1:D:52:HIS:HB2	2.20	0.41
1:D:117:ALA:O	1:D:127:ARG:NH2	2.54	0.41
1:A:217:GLN:O	1:A:226:ALA:HA	2.21	0.41



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASP:OD2	1:C:127:ARG:HD2	2.20	0.41
1:D:331:ASN:HD21	1:D:363:ALA:HA	1.86	0.41
1:B:247:HIS:HA	1:B:264:CYS:HB3	2.02	0.40
1:A:133:ASP:O	1:A:137:ILE:HG13	2.21	0.40
1:A:244:GLU:CG	1:A:247:HIS:HD2	2.35	0.40
1:B:203:GLU:HA	1:B:207:GLY:HA3	2.04	0.40
1:D:91:ARG:NE	1:D:380:ASN:HD21	2.10	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	Perc	entiles
1	А	378/406~(93%)	346 (92%)	25~(7%)	7(2%)	8	20
1	В	378/406~(93%)	353~(93%)	25~(7%)	0	100	100
1	С	378/406~(93%)	344 (91%)	31 (8%)	3~(1%)	19	43
1	D	378/406~(93%)	351 (93%)	24 (6%)	3(1%)	19	43
All	All	1512/1624 (93%)	1394 (92%)	105 (7%)	13 (1%)	17	40

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	290	LEU
1	С	106	SER
1	D	369	GLN
1	А	286	MSE
1	С	294	PRO
1	А	94	ARG
1	D	288	SER
1	А	106	SER



Continued from previous page...

	J	1	1 5
Mol	Chain	\mathbf{Res}	Type
1	А	232	GLY
1	А	271	VAL
1	С	168	PRO
1	D	380	ASN
1	А	382	GLY

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	Perce	entiles
1	А	321/329~(98%)	279~(87%)	42 (13%)	4	10
1	В	321/329~(98%)	276~(86%)	45 (14%)	3	8
1	С	321/329~(98%)	273~(85%)	48 (15%)	3	7
1	D	321/329~(98%)	272~(85%)	49~(15%)	2	7
All	All	1284/1316~(98%)	1100 (86%)	184 (14%)	3	8

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	33	ARG
1	А	47	ILE
1	А	54	MSE
1	А	78	LEU
1	А	82	THR
1	А	88	LEU
1	А	90	LEU
1	А	96	GLU
1	А	99	LEU
1	А	101	LEU
1	А	110	VAL
1	А	116	LEU
1	А	125	LEU
1	А	138	ARG
1	А	143	LEU
1	А	153	LEU



Mol	Chain	Res	Type
1	A	159	THR
1	А	178	LEU
1	A	188	VAL
1	A	213	ARG
1	A	230	THR
1	A	231	ASP
1	A	241	SER
1	A	255	LYS
1	A	265	LEU
1	A	267	THR
1	A	273	SER
1	A	282	LEU
1	A	285	SER
1	A	287	SER
1	A	288	SER
1	A	293	GLN
1	A	295	LEU
1	A	300	LEU
1	A	310	LEU
1	A	326	LEU
1	A	351	LEU
1	A	364	LEU
1	A	384	MSE
1	A	399	LEU
1	A	401	ILE
1	A	405	GLN
1	В	13	ILE
1	В	42	LEU
1	В	78	LEU
1	В	88	LEU
1	В	90	LEU
1	В	101	LEU
1	В	107	LYS
1	В	110	VAL
1	В	115	GLU
1	В	125	LEU
1	В	143	LEU
1	В	144	GLU
1	В	145	ARG
1	В	152	THR
1	В	153	LEU
1	В	178	LEU
			-



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1 B 182 LEU	J
1 B 188 VAI	
1 B 213 ARC	ť
1 B 230 THE	1
1 B 248 THE	{
1 B 250 VAI	_
1 B 255 LYS	5
1 B 265 LEU	J
1 B 268 ILE	
1 B 282 LEU	J
1 B 287 SER	ł
1 B 293 GLN	I
1 B 295 LEU	J
1 B 297 VAI	
1 B 300 LEU	J
1 B 302 GLN	I
1 B 310 LEU	J
1 B 325 ILE	
1 B 334 ASN	I
1 B 336 GLN	I
1 B 351 LEU	J
1 B 364 LEU	J
1 B 370 HIS	
1 B 371 ILE	
1 B 375 SER	ł
1 B 376 THE	1
1 B 399 LEU	J
1 B 400 LEU	J
1 B 405 GLN	1
1 C 12 GLN	1
1 C 16 THE	1
1 C 37 SER	t
1 C 78 LEU	J
1 C 81 GLU	J
1 C 88 LEU	J
1 C 89 SER	t
1 C 90 LEU	J
1 C 101 LEU	J
	ł
$1 \cup 100 SER$	•
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	i
I C 105 SER 1 C 106 SER 1 C 108 LEU	i J



Mol	Chain	Res	Type
1	С	125	LEU
1	C	130	SER
1	C	140	GLN
1	C	141	LYS
1	C	143	LEU
1	С	144	GLU
1	С	145	ARG
1	С	153	LEU
1	С	178	LEU
1	С	184	GLN
1	С	195	ASP
1	С	213	ARG
1	С	230	THR
1	С	265	LEU
1	С	270	SER
1	С	287	SER
1	С	293	GLN
1	С	295	LEU
1	С	298	ASP
1	С	300	LEU
1	С	301	CYS
1	С	309	LEU
1	С	326	LEU
1	С	328	ILE
1	С	340	ILE
1	С	351	LEU
1	С	357	ASP
1	С	361	GLN
1	C	364	LEU
1	С	371	ILE
1	С	372	SER
1	C	376	THR
1	С	399	LEU
1	C	400	LEU
1	С	402	ARG
1	D	13	ILE
1	D	23	ARG
1	D	33	ARG
1	D	35	ASP
1	D	42	LEU
1	D	47	ILE
1	D	54	MSE



Mol	Chain	Res	Type
1	D	62	GLU
1	D	78	LEU
1	D	79	VAL
1	D	81	GLU
1	D	88	LEU
1	D	103	ASP
1	D	108	LEU
1	D	110	VAL
1	D	122	LEU
1	D	125	LEU
1	D	138	ARG
1	D	143	LEU
1	D	153	LEU
1	D	168	PRO
1	D	178	LEU
1	D	184	GLN
1	D	197	SER
1	D	213	ARG
1	D	230	THR
1	D	239	SER
1	D	242	LEU
1	D	255	LYS
1	D	265	LEU
1	D	280	LEU
1	D	282	LEU
1	D	293	GLN
1	D	295	LEU
1	D	298	ASP
1	D	300	LEU
1	D	306	ARG
1	D	310	LEU
1	D	316	THR
1	D	326	LEU
1	D	351	LEU
1	D	360	ARG
1	D	364	LEU
1	D	374	GLU
1	D	375	SER
1	D	381	GLN
1	D	399	LEU
1	D	400	LEU
1	D	402	ARG



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	86	HIS
1	А	131	HIS
1	А	184	GLN
1	А	194	HIS
1	А	279	GLN
1	А	284	GLN
1	А	334	ASN
1	А	405	GLN
1	В	86	HIS
1	В	184	GLN
1	В	193	GLN
1	В	194	HIS
1	В	262	HIS
1	В	334	ASN
1	С	193	GLN
1	С	194	HIS
1	С	279	GLN
1	С	283	ASN
1	С	284	GLN
1	С	334	ASN
1	D	41	GLN
1	D	86	HIS
1	D	185	HIS
1	D	279	GLN
1	D	380	ASN
1	D	381	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 monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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		$OWAB(Å^2)$	Q<0.9
1	А	373/406~(91%)	0.90	50 (13%) 3	2	57, 71, 78, 87	0
1	В	373/406~(91%)	0.36	17 (4%) 32	31	61, 71, 78, 87	0
1	С	373/406~(91%)	0.65	41 (10%) 5	4	61, 71, 77, 84	0
1	D	373/406~(91%)	1.17	89 (23%) 0	0	60, 71, 77, 86	0
All	All	1492/1624~(91%)	0.77	197 (13%) 3	2	57, 71, 78, 87	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	382	GLY	12.6
1	А	62	GLU	11.0
1	В	406	GLY	8.8
1	А	77	GLY	7.9
1	С	406	GLY	7.6
1	D	118	LEU	7.2
1	А	406	GLY	7.1
1	А	61	GLN	6.9
1	А	48	THR	6.5
1	А	45	ALA	6.3
1	А	28	LEU	6.2
1	А	120	ASP	6.2
1	D	123	PRO	6.2
1	D	256	ARG	6.0
1	С	294	PRO	5.9
1	D	253	TYR	5.8
1	А	29	GLY	5.5
1	А	160	GLU	5.4
1	А	63	LEU	5.3
1	D	143	LEU	5.2
1	А	38	ARG	5.1



1Z6R

Mol	Chain	Res	Type	RSRZ
1	D	141	LYS	5.1
1	D	259	CYS	5.1
1	А	46	SER	5.1
1	D	255	LYS	5.1
1	D	406	GLY	5.0
1	А	122	LEU	5.0
1	D	160	GLU	4.9
1	В	63	LEU	4.8
1	D	187	GLY	4.8
1	D	405	GLN	4.7
1	А	121	ASP	4.7
1	А	43	ALA	4.7
1	D	122	LEU	4.5
1	D	369	GLN	4.5
1	А	405	GLN	4.5
1	А	52	HIS	4.4
1	D	21	VAL	4.5
1	D	57	ALA	4.4
1	D	258	TYR	4.4
1	С	309	LEU	4.4
1	D	119	LYS	4.4
1	D	58	HIS	4.4
1	А	292	GLY	4.3
1	D	254	GLY	4.3
1	А	30	PRO	4.3
1	D	63	LEU	4.2
1	А	22	TYR	4.1
1	D	12	GLN	4.1
1	D	56	GLU	4.1
1	D	238	GLY	4.1
1	D	120	ASP	4.1
1	А	44	PRO	4.0
1	D	28	LEU	4.0
1	D	38	ARG	4.0
1	С	369	GLN	4.0
1	С	63	LEU	3.9
1	С	121	ASP	3.9
1	А	119	LYS	3.9
1	С	77	GLY	3.8
1	С	30	PRO	3.8
1	D	44	PRO	3.8
1	А	78	LEU	3.8



Mol	Chain	Res	Type	RSRZ
1	D	111	GLU	3.8
1	D	180	GLU	3.8
1	D	370	HIS	3.7
1	А	166	ARG	3.7
1	D	14	LYS	3.6
1	D	49	LYS	3.6
1	D	77	GLY	3.6
1	В	62	GLU	3.6
1	D	94	ARG	3.4
1	А	57	ALA	3.4
1	D	30	PRO	3.4
1	С	381	GLN	3.4
1	В	121	ASP	3.4
1	D	251	ASP	3.4
1	D	184	GLN	3.3
1	D	142	LYS	3.2
1	D	52	HIS	3.2
1	В	233	HIS	3.2
1	В	306	ARG	3.2
1	А	84	ALA	3.2
1	D	121	ASP	3.1
1	А	12	GLN	3.1
1	D	183	GLU	3.1
1	А	118	LEU	3.1
1	С	293	GLN	3.1
1	А	50	ILE	3.1
1	С	120	ASP	3.1
1	А	49	LYS	3.1
1	D	173	VAL	3.1
1	D	169	PHE	3.0
1	C	238	GLY	3.0
1	D	22	TYR	3.0
1	А	370	HIS	3.0
1	С	12	GLN	3.0
1	С	287	SER	3.0
1	D	381	GLN	2.9
1	D	34	ILE	2.9
1	C	80	VAL	2.9
1	С	41	GLN	2.9
1	С	405	GLN	2.9
1	А	294	PRO	2.9
1	D	228	VAL	2.9



			1	Ζ	6	R
1Z0R	120R	120R		_		_
IZOR	IZOR	1Z0R				
IZOR	IZOR	IZOR				
IZUN	IZUN	IZUN				
120m	12010	IZOIN				
12010	12010	12010				-
12010	12010	12010				
12010	12010	12010		_		_
12010	12010	12010		_		_
12010	12010	12010		_		_
12010	12010	12010		_	-	_
1010	12010	12010		_		_
					_	_

Mol	Chain	Res	Type	RSRZ
1	D	211	GLY	2.9
1	А	58	HIS	2.8
1	А	21	VAL	2.8
1	А	56	GLU	2.8
1	С	370	HIS	2.8
1	D	300	LEU	2.8
1	С	29	GLY	2.8
1	D	92	ILE	2.7
1	D	107	LYS	2.7
1	С	28	LEU	2.7
1	D	140	GLN	2.6
1	С	92	ILE	2.6
1	D	115	GLU	2.6
1	D	135	PHE	2.6
1	D	239	SER	2.6
1	А	59	LEU	2.6
1	D	216	ILE	2.6
1	D	51	VAL	2.6
1	D	90	LEU	2.6
1	С	233	HIS	2.6
1	В	56	GLU	2.6
1	В	88	LEU	2.6
1	С	385	ALA	2.5
1	D	168	PRO	2.5
1	С	40	ALA	2.5
1	D	106	SER	2.5
1	С	115	GLU	2.5
1	С	339	LEU	2.5
1	А	175	GLU	2.5
1	В	115	GLU	2.5
1	C	56	GLU	2.5
1	А	387	ALA	2.5
1	D	222	HIS	2.5
1	D	177	PRO	2.4
1	D	262	HIS	2.4
1	С	59	LEU	2.4
1	D	165	HIS	2.4
1	D	240	SER	2.4
1	С	382	GLY	2.4
1	С	39	LEU	2.4
1	D	161	ASN	2.4
1	D	18	ALA	2.4



1	Ζ	6	F	{

Mol	Chain	Res	Type	RSRZ
1	А	83	GLU	2.4
1	А	180	GLU	2.4
1	А	24	LEU	2.3
1	D	237	ALA	2.3
1	А	60	VAL	2.3
1	С	119	LYS	2.3
1	С	217	GLN	2.3
1	D	229	ILE	2.3
1	D	330	VAL	2.3
1	D	45	ALA	2.3
1	D	95	GLY	2.2
1	С	88	LEU	2.2
1	D	43	ALA	2.2
1	D	210	ARG	2.2
1	D	172	ASP	2.2
1	А	215	VAL	2.2
1	С	311	ALA	2.2
1	В	276	GLU	2.2
1	D	133	ASP	2.2
1	В	184	GLN	2.2
1	С	218	VAL	2.2
1	D	117	ALA	2.2
1	В	151	ILE	2.2
1	С	90	LEU	2.2
1	С	363	ALA	2.2
1	D	33	ARG	2.2
1	D	83	GLU	2.2
1	С	349	ASP	2.2
1	А	293	GLN	2.1
1	В	405	GLN	2.1
1	D	252	PRO	2.1
1	D	40	ALA	2.1
1	В	22	TYR	2.1
1	В	238	GLY	2.1
1	С	216	ILE	2.1
1	А	90	LEU	2.1
1	В	369	GLN	2.1
1	D	186	THR	2.1
1	В	256	ARG	2.1
1	А	88	LEU	2.1
1	С	171	GLU	2.1
1	D	404	LEU	2.1



Mol	Chain	Res	Type	RSRZ
1	А	172	ASP	2.1
1	D	105	SER	2.1
1	D	233	HIS	2.0
1	С	353	PRO	2.0
1	D	17	ASN	2.0
1	А	161	ASN	2.0
1	А	311	ALA	2.0
1	D	114	GLN	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 monosaccharides 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^{th} 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	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
2	ZN	С	503	1/1	0.97	0.07	71,71,71,71	0
2	ZN	D	504	1/1	0.97	0.11	86,86,86,86	0
2	ZN	А	501	1/1	0.98	0.10	$55,\!55,\!55,\!55$	0
2	ZN	В	502	1/1	0.99	0.07	46,46,46,46	0

6.5 Other polymers (i)

There are no such residues in this entry.

