Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2021 – 08:48 AM EDT

PDB ID	:	1Z6R
Title	:	Crystal structure of Mlc from Escherichia coli
Authors	:	Schiefner, A.; Gerber, K.; Seitz, S.; Welte, W.; Diederichs, K.; Boos, W.
Deposited on	:	2005-03-23
Resolution	:	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 (i)) were used in the production of this report:

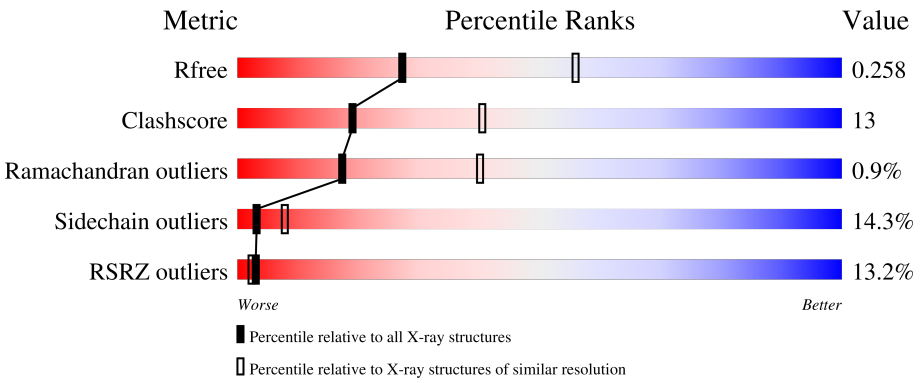
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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-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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
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 chain
1	A	406	12% 64% 24% 6% 6%
1	B	406	4% 60% 29% 5% 6%
1	C	406	10% 56% 33% • • 6%
1	D	406	22% 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.

- Molecule 1 is a protein called Mlc protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	382	2931	1855	514	549	4	9	0	0	0
1	B	382	2931	1855	514	549	4	9	0	0	0
1	C	382	2931	1855	514	549	4	9	0	0	0
1	D	382	2931	1855	514	549	4	9	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	394	MSE	MET	modified residue	UNP P50456
C	1	MSE	MET	modified residue	UNP P50456
C	52	HIS	ARG	engineered mutation	UNP P50456
C	54	MSE	MET	modified residue	UNP P50456
C	167	MSE	MET	modified residue	UNP P50456
C	176	MSE	MET	modified residue	UNP P50456
C	201	MSE	MET	modified residue	UNP P50456
C	286	MSE	MET	modified residue	UNP P50456
C	289	MSE	MET	modified residue	UNP P50456
C	329	MSE	MET	modified residue	UNP P50456
C	384	MSE	MET	modified residue	UNP P50456
C	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).

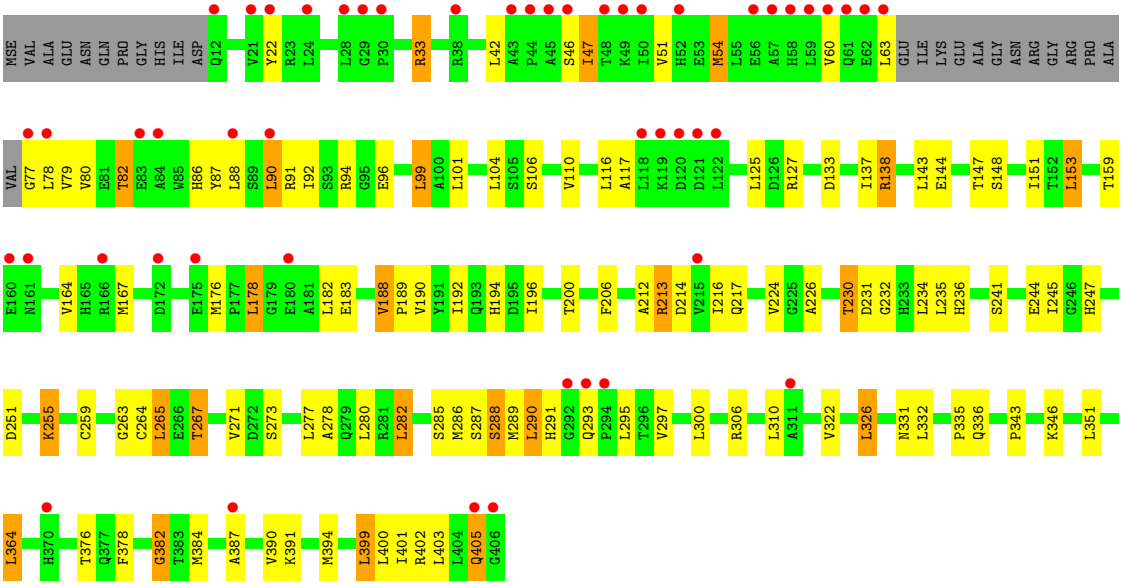
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

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.

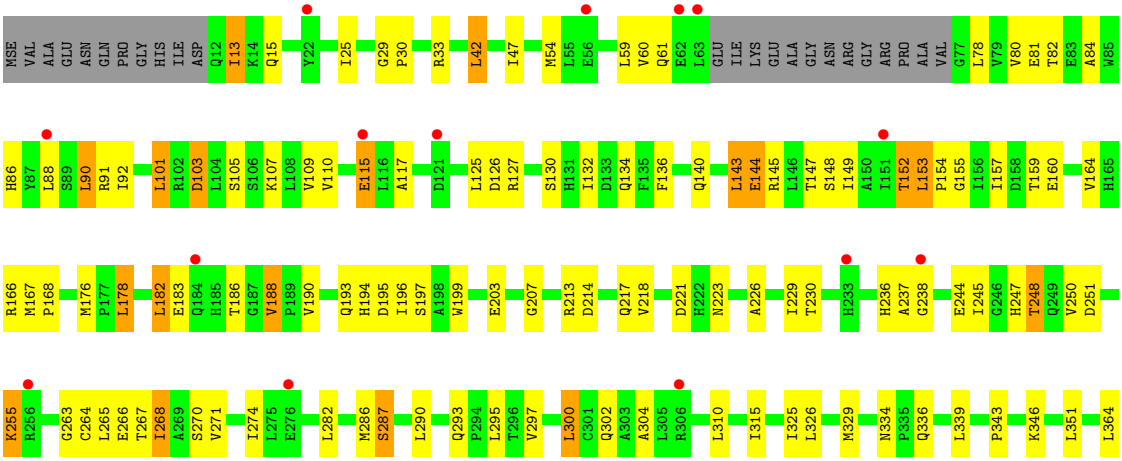
- Molecule 1: Mlc protein

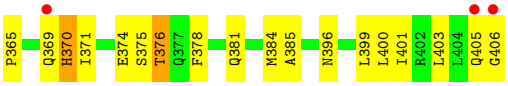
Chain A:



- Molecule 1: Mlc protein

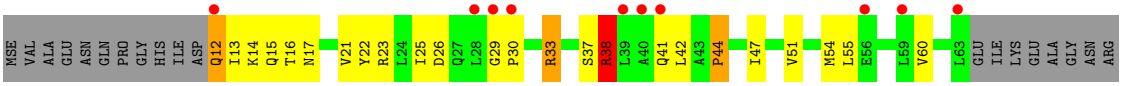
Chain B:

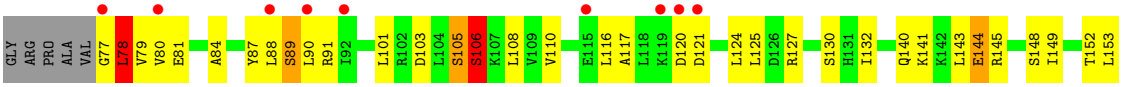


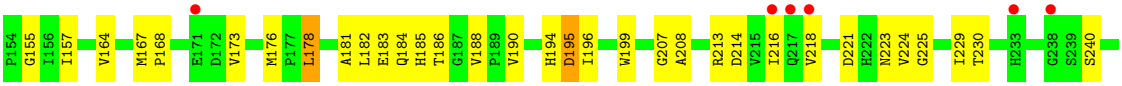


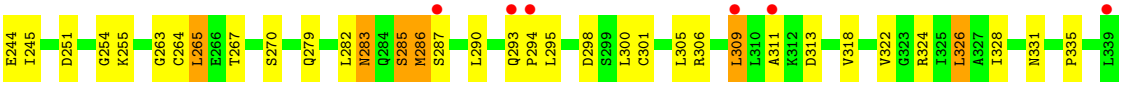
• Molecule 1: Mlc protein

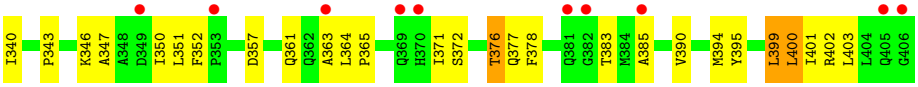
Chain C:





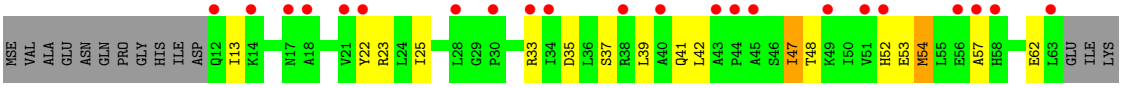


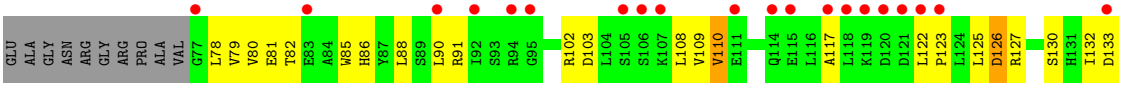


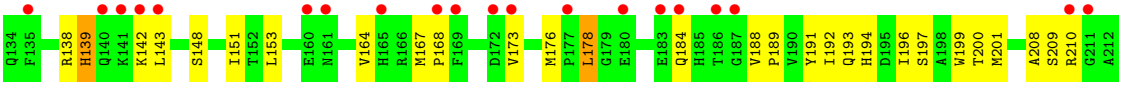


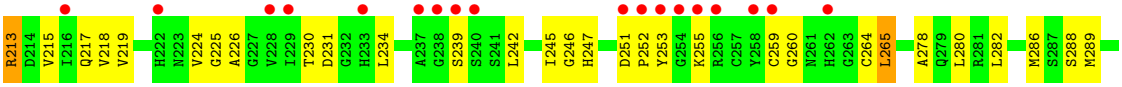
• Molecule 1: Mlc protein

Chain D:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.95Å 74.71Å 154.95Å 90.00° 129.15° 90.00°	Depositor
Resolution (Å)	19.94 – 2.70 19.94 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.94-2.70) 99.0 (19.94-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.263 0.201 , 0.258	Depositor 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/Å^3), B_{sol}(Å^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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.66	5/2969 (0.2%)	0.75	3/4010 (0.1%)
1	B	0.78	1/2969 (0.0%)	0.81	3/4010 (0.1%)
1	C	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	C	0	3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	285	SER	CB-OG	26.01	1.76	1.42
1	C	38	ARG	CZ-NH1	22.97	1.62	1.33
1	B	406	GLY	C-O	16.27	1.49	1.23
1	C	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	A	138	ARG	CZ-NH1	9.77	1.45	1.33
1	C	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

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

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	38	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	C	33	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	A	138	ARG	NE-CZ-NH2	-9.88	115.36	120.30
1	C	44	PRO	O-C-N	7.72	135.05	122.70
1	B	406	GLY	CA-C-O	-6.51	108.88	120.60
1	C	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	A	364	LEU	CA-CB-CG	6.00	129.11	115.30
1	C	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	B	42	LEU	CA-CB-CG	5.54	128.05	115.30
1	C	44	PRO	CA-C-N	-5.34	105.44	117.20
1	B	103	ASP	CB-CA-C	-5.29	99.82	110.40
1	C	286	MSE	CA-C-N	-5.24	105.68	117.20
1	C	324	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	78	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	A	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	C	286	MSE	Mainchain
1	C	38	ARG	Sidechain
1	C	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	A	2931	0	2988	70	0
1	B	2931	0	2988	92	0
1	C	2931	0	2988	88	0
1	D	2931	0	2988	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	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 distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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	Interatomic distance (Å)	Clash 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash 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

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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	Percentiles
1	A	378/406 (93%)	346 (92%)	25 (7%)	7 (2%)	8 20
1	B	378/406 (93%)	353 (93%)	25 (7%)	0	100 100
1	C	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	A	290	LEU
1	C	106	SER
1	D	369	GLN
1	A	286	MSE
1	C	294	PRO
1	A	94	ARG
1	D	288	SER
1	A	106	SER

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Mol	Chain	Res	Type
1	A	232	GLY
1	A	271	VAL
1	C	168	PRO
1	D	380	ASN
1	A	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	Percentiles
1	A	321/329 (98%)	279 (87%)	42 (13%)	4 10
1	B	321/329 (98%)	276 (86%)	45 (14%)	3 8
1	C	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	A	33	ARG
1	A	47	ILE
1	A	54	MSE
1	A	78	LEU
1	A	82	THR
1	A	88	LEU
1	A	90	LEU
1	A	96	GLU
1	A	99	LEU
1	A	101	LEU
1	A	110	VAL
1	A	116	LEU
1	A	125	LEU
1	A	138	ARG
1	A	143	LEU
1	A	153	LEU

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Mol	Chain	Res	Type
1	A	159	THR
1	A	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	B	13	ILE
1	B	42	LEU
1	B	78	LEU
1	B	88	LEU
1	B	90	LEU
1	B	101	LEU
1	B	107	LYS
1	B	110	VAL
1	B	115	GLU
1	B	125	LEU
1	B	143	LEU
1	B	144	GLU
1	B	145	ARG
1	B	152	THR
1	B	153	LEU
1	B	178	LEU

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Mol	Chain	Res	Type
1	B	182	LEU
1	B	188	VAL
1	B	213	ARG
1	B	230	THR
1	B	248	THR
1	B	250	VAL
1	B	255	LYS
1	B	265	LEU
1	B	268	ILE
1	B	282	LEU
1	B	287	SER
1	B	293	GLN
1	B	295	LEU
1	B	297	VAL
1	B	300	LEU
1	B	302	GLN
1	B	310	LEU
1	B	325	ILE
1	B	334	ASN
1	B	336	GLN
1	B	351	LEU
1	B	364	LEU
1	B	370	HIS
1	B	371	ILE
1	B	375	SER
1	B	376	THR
1	B	399	LEU
1	B	400	LEU
1	B	405	GLN
1	C	12	GLN
1	C	16	THR
1	C	37	SER
1	C	78	LEU
1	C	81	GLU
1	C	88	LEU
1	C	89	SER
1	C	90	LEU
1	C	101	LEU
1	C	105	SER
1	C	106	SER
1	C	108	LEU
1	C	110	VAL

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

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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	A	86	HIS
1	A	131	HIS
1	A	184	GLN
1	A	194	HIS
1	A	279	GLN
1	A	284	GLN
1	A	334	ASN
1	A	405	GLN
1	B	86	HIS
1	B	184	GLN
1	B	193	GLN
1	B	194	HIS
1	B	262	HIS
1	B	334	ASN
1	C	193	GLN
1	C	194	HIS
1	C	279	GLN
1	C	283	ASN
1	C	284	GLN
1	C	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, 95th 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	A	373/406 (91%)	0.90	50 (13%)	3	2	57, 71, 78, 87	0
1	B	373/406 (91%)	0.36	17 (4%)	32	31	61, 71, 78, 87	0
1	C	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	A	62	GLU	11.0
1	B	406	GLY	8.8
1	A	77	GLY	7.9
1	C	406	GLY	7.6
1	D	118	LEU	7.2
1	A	406	GLY	7.1
1	A	61	GLN	6.9
1	A	48	THR	6.5
1	A	45	ALA	6.3
1	A	28	LEU	6.2
1	A	120	ASP	6.2
1	D	123	PRO	6.2
1	D	256	ARG	6.0
1	C	294	PRO	5.9
1	D	253	TYR	5.8
1	A	29	GLY	5.5
1	A	160	GLU	5.4
1	A	63	LEU	5.3
1	D	143	LEU	5.2
1	A	38	ARG	5.1

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

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Mol	Chain	Res	Type	RSRZ
1	D	111	GLU	3.8
1	D	180	GLU	3.8
1	D	370	HIS	3.7
1	A	166	ARG	3.7
1	D	14	LYS	3.6
1	D	49	LYS	3.6
1	D	77	GLY	3.6
1	B	62	GLU	3.6
1	D	94	ARG	3.4
1	A	57	ALA	3.4
1	D	30	PRO	3.4
1	C	381	GLN	3.4
1	B	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	B	233	HIS	3.2
1	B	306	ARG	3.2
1	A	84	ALA	3.2
1	D	121	ASP	3.1
1	A	12	GLN	3.1
1	D	183	GLU	3.1
1	A	118	LEU	3.1
1	C	293	GLN	3.1
1	A	50	ILE	3.1
1	C	120	ASP	3.1
1	A	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	A	370	HIS	3.0
1	C	12	GLN	3.0
1	C	287	SER	3.0
1	D	381	GLN	2.9
1	D	34	ILE	2.9
1	C	80	VAL	2.9
1	C	41	GLN	2.9
1	C	405	GLN	2.9
1	A	294	PRO	2.9
1	D	228	VAL	2.9

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

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

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Mol	Chain	Res	Type	RSRZ
1	A	172	ASP	2.1
1	D	105	SER	2.1
1	D	233	HIS	2.0
1	C	353	PRO	2.0
1	D	17	ASN	2.0
1	A	161	ASN	2.0
1	A	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	C	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	A	501	1/1	0.98	0.10	55,55,55,55	0
2	ZN	B	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.