Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 10:26 pm BST

PDB ID	:	2ID0
Title	:	Escherichia coli RNase II
Authors	:	Zuo, Y.; Zhang, J.; Wang, Y.; Malhotra, A.
Deposited on	:	2006-09-13
Resolution	:	2.35 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 ⓘ symbol.

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

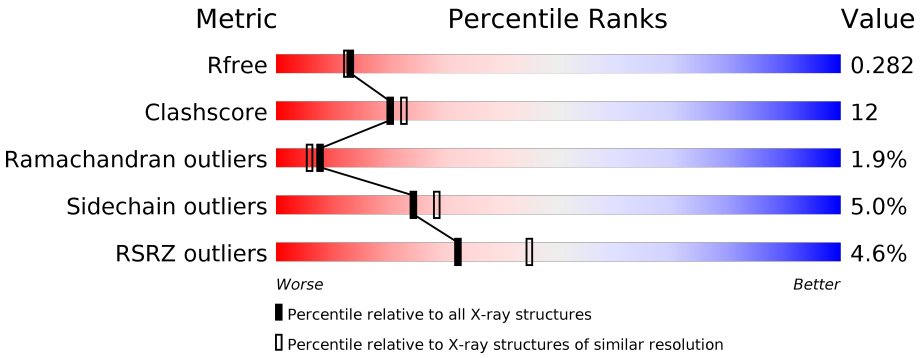
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 >=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	644	12% 64% 31%
1	B	644	% 74% 24%
1	C	644	% 75% 21%
1	D	644	4% 68% 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19820 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 Exoribonuclease 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	636	Total	C	N	O	S	Se	0	0	0
			4838	3078	860	879	7	14			
1	B	636	Total	C	N	O	S	Se	0	0	0
			4937	3128	879	909	7	14			
1	C	636	Total	C	N	O	S	Se	0	0	0
			4930	3129	876	904	7	14			
1	D	636	Total	C	N	O	S	Se	0	0	0
			4824	3072	853	878	7	14			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	51	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	55	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	132	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	182	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	208	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	261	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	286	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	393	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	417	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	505	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	531	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	540	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	576	MSE	MET	MODIFIED RESIDUE	UNP P30850
A	633	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	1	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	51	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	55	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	132	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	182	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	208	MSE	MET	MODIFIED RESIDUE	UNP P30850

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Chain	Residue	Modelled	Actual	Comment	Reference
B	261	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	286	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	393	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	417	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	505	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	531	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	540	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	576	MSE	MET	MODIFIED RESIDUE	UNP P30850
B	633	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	1	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	51	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	55	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	132	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	182	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	208	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	261	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	286	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	393	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	417	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	505	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	531	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	540	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	576	MSE	MET	MODIFIED RESIDUE	UNP P30850
C	633	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	1	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	51	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	55	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	132	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	182	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	208	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	261	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	286	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	393	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	417	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	505	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	531	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	540	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	576	MSE	MET	MODIFIED RESIDUE	UNP P30850
D	633	MSE	MET	MODIFIED RESIDUE	UNP P30850

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is water.

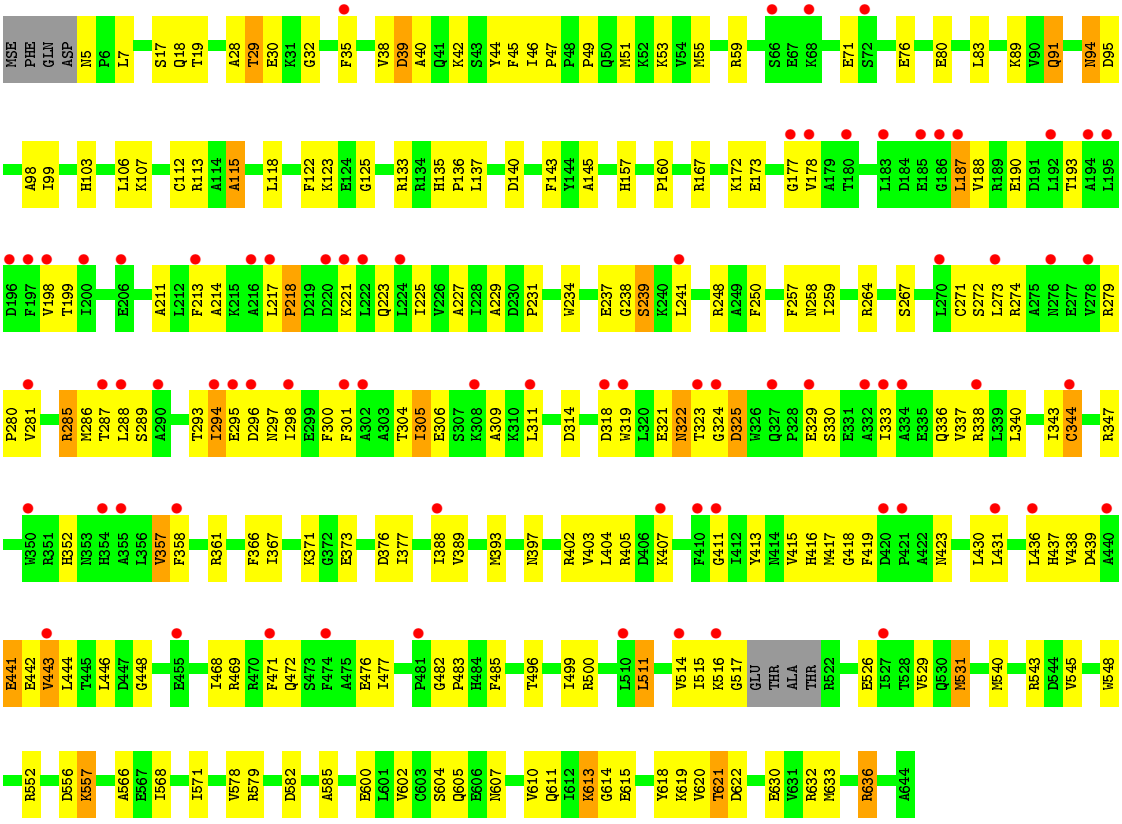
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	50	Total O 50 50	0	0
3	B	96	Total O 96 96	0	0
3	C	82	Total O 82 82	0	0
3	D	59	Total O 59 59	0	0

3 Residue-property plots (i)

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

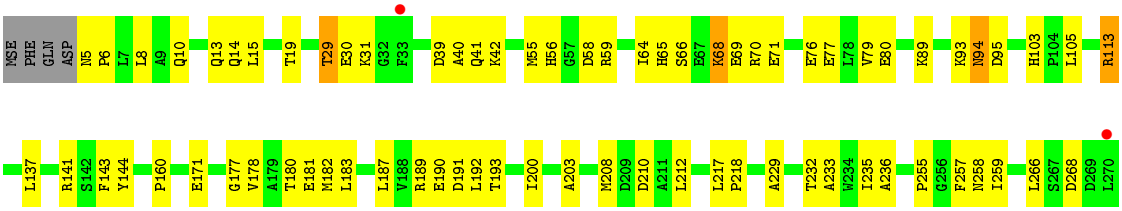
- Molecule 1: Exoribonuclease 2

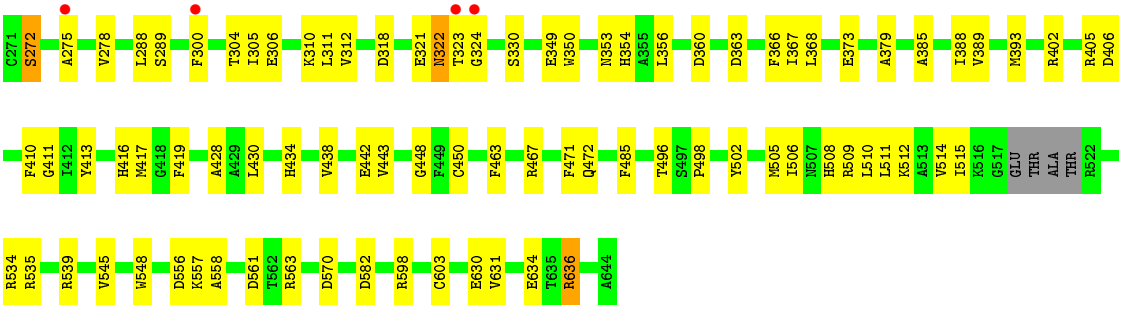
Chain A:



- Molecule 1: Exoribonuclease 2

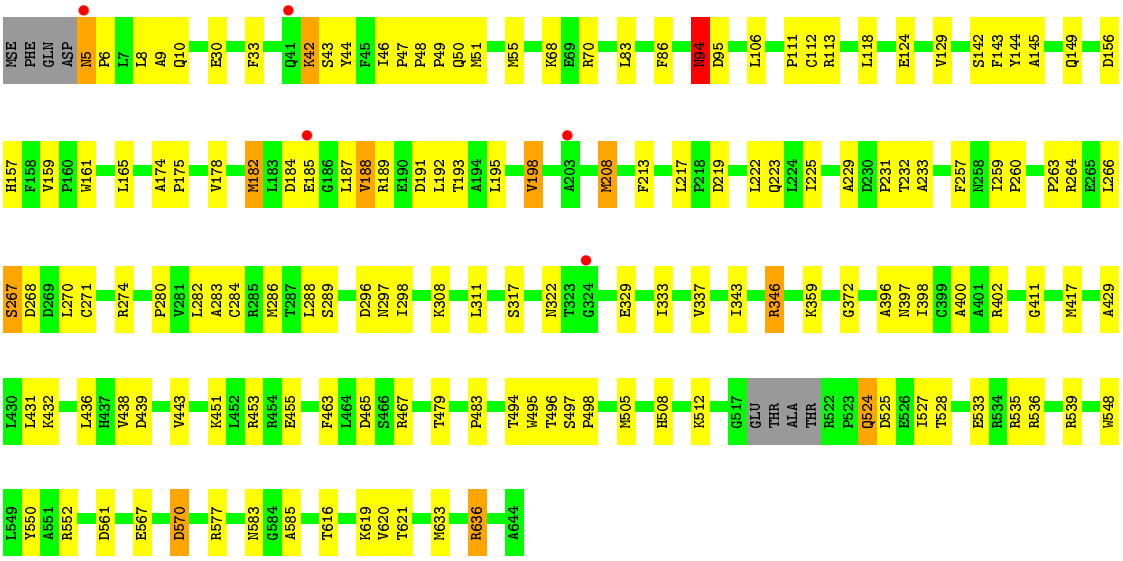
Chain B:





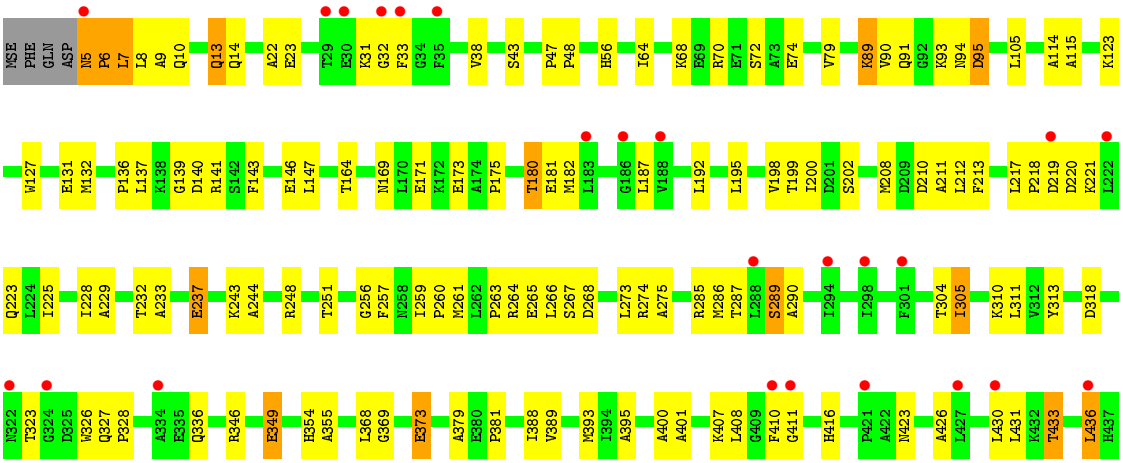
• Molecule 1: Exoribonuclease 2

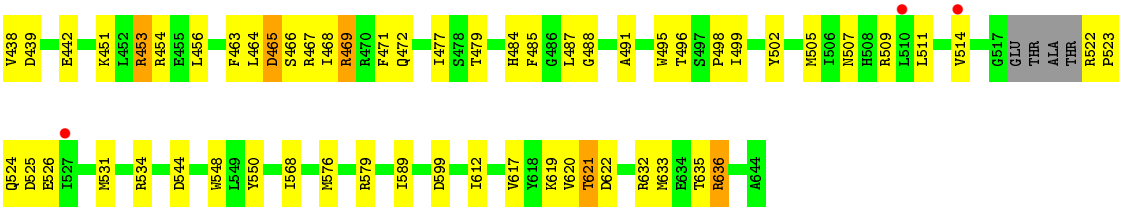
Chain C:



• Molecule 1: Exoribonuclease 2

Chain D:




V438
D439
E442
K451
L452
R453
R454
E455
L456
F463
L464
D465
S466
R467
I468
R469
R470
F471
Q472
I477
S478
T479
H484
F485
G486
L487
G488
A491
W495
T496
S497
P498
I499
Y502
M505
I506
N507
H508
R509
L510
L511
V514
G517
GLU
THR
ALA
THR
R522
P523
Q524
D525
E526
I527
M531
R534
D544
W548
L549
V550
I568
M576
R579
I589
D599
I612
V617
Y618
K619
V620
T621
D622
R632
M633
E634
T635
R636
A644

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.76Å 118.43Å 122.38Å 107.80° 98.36° 91.40°	Depositor
Resolution (Å)	17.95 – 2.35 17.95 – 2.35	Depositor EDS
% Data completeness (in resolution range)	82.3 (17.95-2.35) 82.4 (17.95-2.35)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	7.80 (at 2.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.286 0.221 , 0.282	Depositor DCC
R_{free} test set	5045 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19820	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.14% 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

5.1 Standard geometry

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

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	0.81	9/4925 (0.2%)	0.78	2/6674 (0.0%)
1	B	0.83	3/5025 (0.1%)	0.80	3/6800 (0.0%)
1	C	0.80	0/5018	0.80	2/6788 (0.0%)
1	D	0.86	8/4911 (0.2%)	0.83	3/6659 (0.0%)
All	All	0.82	20/19879 (0.1%)	0.80	10/26921 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ARG	CZ-NH1	16.16	1.54	1.33
1	B	190	GLU	CD-OE1	15.89	1.43	1.25
1	B	190	GLU	CD-OE2	15.08	1.42	1.25
1	D	5	ASN	CG-ND2	14.79	1.69	1.32
1	D	285	ARG	NE-CZ	13.06	1.50	1.33
1	D	14	GLN	C-O	12.78	1.47	1.23
1	A	301	PHE	CE2-CZ	8.16	1.52	1.37
1	A	285	ARG	CZ-NH2	6.98	1.42	1.33
1	A	301	PHE	CG-CD2	6.90	1.49	1.38
1	D	13	GLN	CD-OE1	6.37	1.38	1.24
1	D	5	ASN	N-CA	6.21	1.58	1.46
1	A	188	VAL	C-O	6.12	1.34	1.23
1	D	14	GLN	C-N	6.08	1.48	1.34
1	A	517	GLY	CA-C	5.73	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	LYS	C-O	5.19	1.33	1.23
1	B	603	CYS	CB-SG	-5.18	1.73	1.81
1	A	298	ILE	C-N	5.16	1.46	1.34
1	D	550	TYR	CD1-CE1	5.07	1.47	1.39
1	D	13	GLN	CG-CD	5.06	1.62	1.51
1	A	285	ARG	CD-NE	5.01	1.54	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	285	ARG	NE-CZ-NH2	-15.12	112.74	120.30
1	A	285	ARG	NE-CZ-NH2	-13.85	113.38	120.30
1	D	285	ARG	NE-CZ-NH1	12.31	126.46	120.30
1	C	535	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	B	58	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	8	LEU	CB-CG-CD2	-6.81	99.42	111.00
1	B	8	LEU	CA-CB-CG	6.36	129.92	115.30
1	C	535	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	301	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	D	599	ASP	CB-CG-OD1	5.47	123.22	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	ASN	Peptide

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	4838	0	4707	142	0
1	B	4937	0	4850	98	0
1	C	4930	0	4860	99	0
1	D	4824	0	4698	142	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	50	0	0	5	0
3	B	96	0	0	3	0
3	C	82	0	0	2	0
3	D	59	0	0	3	0
All	All	19820	0	19115	481	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 12.

All (481) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:ASN:ND2	1:D:5:ASN:CG	1.69	1.44
1:A:431:LEU:HD13	1:A:438:VAL:HG21	1.30	1.12
1:D:217:LEU:HB3	1:D:218:PRO:HD2	1.30	1.07
1:D:5:ASN:HB2	1:D:6:PRO:HD3	1.44	0.99
1:D:393:MSE:SE	1:D:496:THR:HG21	2.16	0.95
1:A:439:ASP:O	1:A:443:VAL:HG23	1.69	0.93
1:D:275:ALA:H	1:D:310:LYS:HE3	1.34	0.90
1:B:103:HIS:HE1	1:B:105:LEU:HD12	1.38	0.88
1:A:59:ARG:HH21	1:A:80:GLU:HG2	1.38	0.88
1:D:5:ASN:HB2	1:D:6:PRO:CD	2.06	0.86
1:D:217:LEU:HB3	1:D:218:PRO:CD	2.05	0.84
1:C:68:LYS:HB3	1:C:70:ARG:O	1.76	0.84
1:B:582:ASP:OD2	3:B:1044:HOH:O	1.96	0.83
1:D:407:LYS:HG3	1:D:514:VAL:HG13	1.61	0.82
1:B:217:LEU:HB3	1:B:218:PRO:HD2	1.61	0.81
1:B:416:HIS:HB3	1:B:485:PHE:H	1.45	0.81
1:A:115:ALA:O	3:A:1051:HOH:O	1.99	0.80
1:A:318:ASP:HB3	1:A:323:THR:HG21	1.64	0.79
1:D:182:MSE:HE2	1:D:233:ALA:HB1	1.64	0.78
1:A:264:ARG:HA	1:A:267:SER:OG	1.84	0.77
1:C:182:MSE:HE3	1:C:233:ALA:HB1	1.68	0.76
1:C:451:LYS:O	1:C:455:GLU:HG3	1.85	0.76
1:A:430:LEU:HD22	1:A:471:PHE:HE1	1.51	0.76
1:A:403:VAL:HG13	1:A:407:LYS:HE3	1.68	0.75
1:D:208:MSE:HE3	1:D:310:LYS:HE2	1.69	0.75
1:B:180:THR:HG22	1:B:181:GLU:H	1.52	0.74
1:D:318:ASP:HB3	1:D:323:THR:HB	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:ALA:H	1:D:310:LYS:CE	2.00	0.74
1:D:379:ALA:O	1:D:381:PRO:HD3	1.88	0.74
1:D:416:HIS:HB3	1:D:485:PHE:H	1.51	0.74
1:B:498:PRO:HG3	1:B:508:HIS:NE2	2.01	0.74
1:B:182:MSE:HE3	1:B:233:ALA:HB1	1.70	0.74
1:D:393:MSE:SE	1:D:496:THR:CG2	2.85	0.74
1:C:182:MSE:CE	1:C:233:ALA:HB1	2.18	0.73
1:D:469:ARG:HA	1:D:472:GLN:HE21	1.51	0.73
1:A:620:VAL:O	1:A:621:THR:HB	1.88	0.73
1:B:39:ASP:HB3	1:B:42:LYS:HB3	1.70	0.72
1:A:630:GLU:CD	1:A:632:ARG:HE	1.93	0.71
1:B:39:ASP:OD1	1:B:40:ALA:N	2.23	0.71
1:A:55:MSE:SE	1:A:83:LEU:HD12	2.40	0.71
1:B:217:LEU:HB3	1:B:218:PRO:CD	2.21	0.70
1:D:198:VAL:HG22	1:D:199:THR:N	2.06	0.70
1:C:182:MSE:HE3	1:C:233:ALA:CB	2.22	0.70
1:D:93:LYS:HG2	1:D:94:ASN:H	1.55	0.70
1:A:468:ILE:O	1:A:471:PHE:HB2	1.92	0.70
1:D:439:ASP:HB3	1:D:442:GLU:HB2	1.72	0.70
1:B:305:ILE:HG22	1:B:306:GLU:N	2.07	0.69
1:B:76:GLU:HG2	1:B:77:GLU:HG3	1.74	0.68
1:A:214:ALA:HA	1:A:223:GLN:O	1.94	0.68
1:A:29:THR:HG22	1:A:30:GLU:H	1.57	0.68
1:B:318:ASP:HB3	1:B:323:THR:HB	1.75	0.68
1:A:611:GLN:HA	1:A:615:GLU:O	1.93	0.68
1:B:417:MSE:HA	1:B:417:MSE:HE2	1.76	0.68
1:D:484:HIS:CE1	1:D:487:LEU:HG	2.28	0.68
1:B:598:ARG:NH1	3:B:1073:HOH:O	2.27	0.67
1:C:525:ASP:O	1:C:528:THR:HG22	1.94	0.67
1:D:132:MSE:CE	1:D:143:PHE:HD2	2.08	0.67
1:A:411:GLY:HA3	1:A:413:TYR:HE1	1.58	0.67
1:D:463:PHE:CE2	1:D:467:ARG:HD2	2.29	0.67
1:D:453:ARG:HD3	1:D:456:LEU:HD12	1.76	0.67
1:A:397:ASN:HD21	1:A:496:THR:HB	1.60	0.66
1:D:198:VAL:HG21	1:D:311:LEU:CD1	2.25	0.66
1:B:511:LEU:O	1:B:514:VAL:HG12	1.96	0.66
1:A:39:ASP:OD1	1:A:42:LYS:HB2	1.96	0.66
1:B:13:GLN:HG3	1:B:14:GLN:HG2	1.77	0.66
1:C:55:MSE:HE3	1:C:143:PHE:CE2	2.31	0.65
1:D:290:ALA:O	1:D:346:ARG:HD2	1.96	0.65
1:D:431:LEU:HD22	1:D:436:LEU:HD22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:ALA:HA	1:D:488:GLY:O	1.96	0.65
1:A:319:TRP:HH2	1:A:338:ARG:HG3	1.62	0.64
1:A:411:GLY:HA3	1:A:413:TYR:CE1	2.32	0.64
1:A:53:LYS:HG2	1:A:137:LEU:HD23	1.80	0.64
1:D:423:ASN:HB3	1:D:471:PHE:HD2	1.64	0.63
1:A:38:VAL:HB	1:A:42:LYS:HB3	1.79	0.63
1:D:132:MSE:HE1	1:D:143:PHE:HD2	1.63	0.63
1:B:416:HIS:HB3	1:B:485:PHE:N	2.14	0.63
1:A:604:SER:OG	1:A:607:ASN:HB2	1.99	0.63
1:C:161:TRP:O	1:C:165:LEU:HD12	1.99	0.63
1:D:430:LEU:O	1:D:433:THR:HB	1.99	0.62
1:D:182:MSE:HE2	1:D:233:ALA:CB	2.29	0.61
1:A:571:ILE:HD13	1:A:610:VAL:HG23	1.82	0.61
1:A:499:ILE:HG23	1:A:500:ARG:NE	2.16	0.61
1:A:340:LEU:HA	1:A:343:ILE:HD12	1.83	0.61
1:D:5:ASN:CB	1:D:6:PRO:CD	2.78	0.61
1:B:512:LYS:HA	1:B:515:ILE:HD12	1.80	0.61
1:C:498:PRO:HG3	1:C:508:HIS:CE1	2.36	0.61
1:A:431:LEU:HD22	1:A:436:LEU:HD23	1.83	0.61
1:A:199:THR:O	1:A:311:LEU:HB2	2.01	0.61
1:C:175:PRO:HG2	1:C:263:PRO:HD3	1.84	0.60
1:C:561:ASP:OD1	3:C:1048:HOH:O	2.15	0.60
1:D:620:VAL:O	1:D:621:THR:HB	2.01	0.60
1:A:371:LYS:HE2	1:A:373:GLU:HB2	1.82	0.60
1:B:356:LEU:HD21	1:B:450:CYS:HA	1.84	0.60
1:C:5:ASN:HB2	1:C:6:PRO:CD	2.32	0.60
1:C:174:ALA:HB2	1:C:260:PRO:HG2	1.83	0.59
1:B:208:MSE:HE3	1:B:310:LYS:HG2	1.84	0.59
1:A:294:ILE:HD12	1:A:294:ILE:H	1.67	0.59
1:D:198:VAL:CG2	1:D:199:THR:N	2.65	0.59
1:A:213:PHE:HD2	1:A:225:ILE:HD12	1.66	0.59
1:A:630:GLU:OE2	1:A:632:ARG:NE	2.32	0.59
1:B:305:ILE:CG2	1:B:306:GLU:N	2.65	0.59
1:C:229:ALA:HB1	1:C:271:CYS:HB3	1.85	0.59
1:B:535:ARG:O	1:B:539:ARG:HG3	2.03	0.59
1:A:568:ILE:HD12	1:A:622:ASP:HB2	1.85	0.59
1:C:439:ASP:O	1:C:443:VAL:HG23	2.03	0.58
1:D:633:MSE:HG2	3:D:1015:HOH:O	2.03	0.58
1:B:389:VAL:O	1:B:393:MSE:HG2	2.03	0.58
1:A:619:LYS:HE2	1:A:622:ASP:OD1	2.03	0.58
1:C:189:ARG:HH21	1:C:280:PRO:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:SER:O	1:A:272:SER:HB2	2.04	0.58
1:D:257:PHE:CE2	1:D:259:ILE:HD11	2.39	0.58
1:D:507:ASN:O	1:D:511:LEU:HB2	2.04	0.57
1:C:195:LEU:HD22	1:C:213:PHE:CZ	2.38	0.57
1:D:213:PHE:CD2	1:D:225:ILE:HD12	2.40	0.57
1:A:177:GLY:HA2	1:A:241:LEU:HD21	1.85	0.57
1:A:198:VAL:HG12	1:A:309:ALA:HB3	1.87	0.57
1:D:5:ASN:ND2	1:D:5:ASN:CB	2.65	0.57
1:C:329:GLU:O	1:C:329:GLU:HG3	2.03	0.57
1:C:616:THR:HG21	1:C:619:LYS:HE3	1.86	0.57
1:A:367:ILE:HD12	1:A:376:ASP:HB3	1.87	0.56
1:C:47:PRO:C	1:C:49:PRO:HD2	2.25	0.56
1:A:403:VAL:O	1:A:407:LYS:HG2	2.05	0.56
1:C:229:ALA:O	1:C:231:PRO:HD3	2.06	0.56
1:C:189:ARG:NH2	1:C:280:PRO:HB2	2.21	0.56
1:A:415:VAL:HG12	1:A:482:GLY:HA3	1.88	0.56
1:B:556:ASP:OD1	1:B:557:LYS:NZ	2.37	0.56
1:B:305:ILE:CG2	1:B:306:GLU:H	2.19	0.56
1:B:113:ARG:CZ	1:B:113:ARG:HB2	2.35	0.55
1:A:439:ASP:OD1	1:A:441:GLU:HB3	2.06	0.55
1:C:296:ASP:O	1:C:298:ILE:N	2.35	0.55
1:D:524:GLN:C	1:D:526:GLU:H	2.08	0.55
1:C:5:ASN:HB2	1:C:6:PRO:HD3	1.88	0.55
1:D:568:ILE:HD12	1:D:622:ASP:HB2	1.88	0.55
1:B:278:VAL:HG13	1:B:304:THR:HG22	1.89	0.55
1:A:419:PHE:HA	1:A:472:GLN:HA	1.87	0.54
1:D:416:HIS:HB3	1:D:485:PHE:N	2.19	0.54
1:D:400:ALA:HB2	1:D:495:TRP:CD1	2.41	0.54
1:D:408:LEU:HB2	1:D:410:PHE:H	1.72	0.54
1:C:68:LYS:HG3	1:C:70:ARG:H	1.71	0.54
1:D:93:LYS:HG2	1:D:94:ASN:N	2.21	0.54
1:C:174:ALA:CB	1:C:260:PRO:HG2	2.38	0.54
1:A:103:HIS:HB3	1:A:106:LEU:HD12	1.90	0.54
1:D:23:GLU:O	1:D:38:VAL:HG13	2.07	0.54
1:B:442:GLU:O	1:B:448:GLY:HA3	2.07	0.54
1:B:141:ARG:O	1:B:141:ARG:HG2	2.07	0.54
1:C:431:LEU:HD13	1:C:438:VAL:HG21	1.89	0.54
1:A:294:ILE:HD11	1:A:347:ARG:HH12	1.72	0.53
1:D:198:VAL:HG21	1:D:311:LEU:HD12	1.89	0.53
1:D:208:MSE:HB3	1:D:273:LEU:HB2	1.91	0.53
1:A:477:ILE:HD13	1:A:531:MSE:HE2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:GLU:O	1:D:248:ARG:NH2	2.36	0.53
1:D:423:ASN:HB3	1:D:471:PHE:CD2	2.44	0.53
1:D:620:VAL:O	1:D:621:THR:CB	2.57	0.53
1:B:463:PHE:CZ	1:B:467:ARG:HD3	2.44	0.53
1:D:175:PRO:O	1:D:263:PRO:HG3	2.09	0.53
1:D:89:LYS:HD3	1:D:127:TRP:CZ2	2.43	0.53
1:A:257:PHE:CE2	1:A:259:ILE:HD11	2.43	0.53
1:A:272:SER:O	1:A:279:ARG:HD2	2.09	0.53
1:A:47:PRO:HB2	1:A:49:PRO:HD2	1.91	0.53
1:C:431:LEU:HD22	1:C:436:LEU:HD23	1.91	0.53
1:A:211:ALA:HB3	1:A:227:ALA:HB3	1.90	0.53
1:C:400:ALA:HB2	1:C:495:TRP:CD1	2.44	0.53
1:A:279:ARG:HH11	1:A:280:PRO:HD2	1.74	0.53
1:C:217:LEU:HD11	1:C:223:GLN:HB2	1.91	0.53
1:B:208:MSE:CE	1:B:310:LYS:HG2	2.39	0.53
1:C:533:GLU:OE1	1:C:536:ARG:NH2	2.42	0.53
1:D:463:PHE:CZ	1:D:467:ARG:HD2	2.43	0.52
1:B:6:PRO:O	1:B:10:GLN:HG3	2.09	0.52
1:D:136:PRO:HA	1:D:141:ARG:O	2.09	0.52
1:A:118:LEU:HD21	1:A:122:PHE:CE1	2.45	0.52
1:A:446:LEU:HG	1:A:485:PHE:CZ	2.45	0.52
1:C:548:TRP:HA	1:C:636:ARG:HG2	1.90	0.52
1:C:620:VAL:O	1:C:621:THR:HB	2.09	0.52
1:B:366:PHE:HB3	1:B:368:LEU:HD21	1.92	0.52
1:A:352:HIS:HA	1:A:357:VAL:HG22	1.90	0.52
1:A:611:GLN:NE2	1:A:614:GLY:O	2.42	0.52
1:A:29:THR:HG22	1:A:30:GLU:HG3	1.92	0.52
1:C:5:ASN:HD21	1:C:8:LEU:H	1.57	0.52
1:A:431:LEU:HB3	1:A:436:LEU:HB3	1.92	0.52
1:D:612:ILE:HD12	1:D:617:VAL:HG21	1.92	0.52
1:B:321:GLU:O	1:B:322:ASN:CB	2.58	0.52
1:C:208:MSE:HE1	1:C:274:ARG:HA	1.91	0.52
1:C:5:ASN:ND2	1:C:8:LEU:H	2.08	0.51
1:D:251:THR:HG23	1:D:260:PRO:HA	1.91	0.51
1:D:401:ALA:HB1	1:D:491:ALA:HB1	1.92	0.51
1:A:579:ARG:HA	1:A:585:ALA:O	2.11	0.51
1:B:203:ALA:HB2	1:B:312:VAL:HG22	1.91	0.51
1:C:286:MSE:HE1	1:C:396:ALA:HA	1.92	0.51
1:D:438:VAL:HG22	1:D:439:ASP:N	2.26	0.51
1:D:465:ASP:O	1:D:468:ILE:HG12	2.09	0.51
1:A:227:ALA:HB1	1:A:281:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:PHE:CE2	1:A:377:ILE:HD13	2.45	0.51
1:D:115:ALA:HA	1:D:146:GLU:OE2	2.11	0.51
1:C:174:ALA:HB2	1:C:260:PRO:CG	2.41	0.51
1:D:389:VAL:O	1:D:393:MSE:HG2	2.11	0.51
1:B:305:ILE:HG22	1:B:306:GLU:H	1.76	0.51
1:C:188:VAL:O	1:C:188:VAL:HG12	2.11	0.51
1:D:208:MSE:HB2	1:D:273:LEU:H	1.76	0.51
1:B:59:ARG:HG2	1:B:79:VAL:HB	1.92	0.50
1:D:579:ARG:NH2	3:D:1041:HOH:O	2.32	0.50
1:C:438:VAL:CG1	1:C:443:VAL:CG2	2.89	0.50
1:D:304:THR:C	1:D:305:ILE:HG12	2.32	0.50
1:D:632:ARG:HB2	1:D:635:THR:CG2	2.41	0.50
1:A:393:MSE:SE	1:A:496:THR:OG1	2.79	0.50
1:C:417:MSE:HE1	1:C:483:PRO:HD2	1.94	0.50
1:D:408:LEU:HB3	1:D:410:PHE:CD1	2.47	0.50
1:B:275:ALA:HB2	1:B:310:LYS:HG3	1.93	0.50
1:A:330:SER:HB2	1:A:333:ILE:HG12	1.94	0.50
1:A:39:ASP:CG	1:A:40:ALA:N	2.64	0.50
1:B:428:ALA:HA	1:B:438:VAL:HG12	1.94	0.50
1:D:217:LEU:CD1	1:D:287:THR:HG23	2.42	0.50
1:D:286:MSE:SE	1:D:395:ALA:HB1	2.62	0.49
1:A:571:ILE:O	1:A:605:GLN:HA	2.12	0.49
1:D:180:THR:HG22	1:D:181:GLU:H	1.77	0.49
1:A:407:LYS:HG3	1:A:514:VAL:HG22	1.94	0.49
1:C:112:CYS:HA	1:C:145:ALA:O	2.12	0.49
1:D:451:LYS:HA	1:D:454:ARG:HE	1.78	0.49
1:D:477:ILE:HD13	1:D:531:MSE:HE2	1.95	0.49
1:A:213:PHE:CD2	1:A:225:ILE:HD12	2.46	0.49
1:B:235:ILE:HD11	1:B:266:LEU:CD2	2.43	0.49
1:C:397:ASN:OD1	1:C:494:THR:HA	2.12	0.49
1:C:46:ILE:HG22	1:C:50:GLN:HB2	1.94	0.49
1:B:419:PHE:HD2	1:B:471:PHE:O	1.94	0.49
1:D:198:VAL:CG2	1:D:199:THR:H	2.26	0.49
1:D:275:ALA:N	1:D:310:LYS:HE3	2.16	0.49
1:B:561:ASP:HB2	1:B:563:ARG:NH2	2.27	0.49
1:C:570:ASP:OD2	1:C:577:ARG:HD3	2.13	0.49
1:D:171:GLU:CD	1:D:171:GLU:H	2.16	0.49
1:D:200:ILE:HG22	1:D:313:TYR:CE2	2.47	0.49
1:A:112:CYS:HA	1:A:145:ALA:O	2.13	0.49
1:A:431:LEU:HD13	1:A:438:VAL:CG2	2.21	0.49
1:B:55:MSE:HE3	1:B:143:PHE:CE2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:GLN:O	1:B:13:GLN:HG2	2.13	0.48
1:D:213:PHE:HA	1:D:336:GLN:OE1	2.13	0.48
1:A:89:LYS:HZ2	1:A:89:LYS:HB3	1.78	0.48
1:A:229:ALA:O	1:A:231:PRO:HD3	2.13	0.48
1:D:274:ARG:HA	1:D:310:LYS:HE2	1.96	0.48
1:B:300:PHE:CD2	1:B:511:LEU:HD22	2.48	0.48
1:A:300:PHE:O	1:A:515:ILE:HG12	2.13	0.48
1:B:323:THR:OG1	1:B:324:GLY:N	2.47	0.48
1:C:55:MSE:HG3	1:C:106:LEU:HD22	1.94	0.48
1:D:22:ALA:HB3	1:D:64:ILE:HD11	1.95	0.48
1:D:182:MSE:CE	1:D:233:ALA:CB	2.92	0.48
1:A:59:ARG:NH2	1:A:80:GLU:HG2	2.17	0.48
1:A:91:GLN:NE2	1:A:98:ALA:HB3	2.29	0.48
1:C:142:SER:HB3	3:C:1055:HOH:O	2.13	0.48
1:C:33:PHE:HB3	1:C:48:PRO:HD3	1.95	0.48
1:D:632:ARG:HB2	1:D:635:THR:HG22	1.96	0.48
1:B:191:ASP:O	1:B:193:THR:N	2.43	0.48
1:D:139:GLY:O	1:D:140:ASP:HB2	2.14	0.48
1:C:453:ARG:HH22	1:C:465:ASP:CG	2.17	0.48
1:A:135:HIS:CE1	1:A:137:LEU:HB2	2.49	0.47
1:A:389:VAL:O	1:A:393:MSE:HG2	2.14	0.47
1:A:468:ILE:HG13	1:A:469:ARG:N	2.29	0.47
1:C:156:ASP:HB3	1:C:159:VAL:HG23	1.96	0.47
1:A:113:ARG:HD2	3:A:1037:HOH:O	2.14	0.47
1:A:333:ILE:O	1:A:337:VAL:HG23	2.14	0.47
1:A:526:GLU:O	1:A:529:VAL:HB	2.14	0.47
1:B:278:VAL:HA	1:B:305:ILE:O	2.14	0.47
1:C:129:VAL:HB	1:C:149:GLN:HB3	1.96	0.47
1:D:576:MSE:HE2	1:D:589:ILE:HD12	1.96	0.47
1:D:7:LEU:O	1:D:10:GLN:HB2	2.14	0.47
1:A:402:ARG:O	1:A:405:ARG:HB3	2.14	0.47
1:A:442:GLU:HG2	1:A:448:GLY:HA3	1.96	0.47
1:A:600:GLU:HG2	1:A:613:LYS:HG3	1.96	0.47
1:B:548:TRP:HA	1:B:636:ARG:HG2	1.96	0.47
1:C:266:LEU:HD23	1:C:270:LEU:HD12	1.96	0.47
1:C:463:PHE:CZ	1:C:467:ARG:HD3	2.50	0.47
1:A:32:GLY:O	1:A:51:MSE:HG3	2.14	0.47
1:B:257:PHE:CE2	1:B:259:ILE:HD11	2.48	0.47
1:A:118:LEU:HD21	1:A:122:PHE:HE1	1.79	0.47
1:A:234:TRP:HH2	1:A:280:PRO:CG	2.27	0.47
1:A:28:ALA:HB2	1:A:51:MSE:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:VAL:HG22	1:B:443:VAL:HG13	1.97	0.47
1:A:250:PHE:HE1	1:A:531:MSE:O	1.97	0.47
1:B:182:MSE:HE2	1:B:182:MSE:HB3	1.84	0.47
1:B:65:HIS:O	1:B:71:GLU:HA	2.15	0.47
1:D:327:GLN:HG2	1:D:328:PRO:HD2	1.95	0.47
1:A:39:ASP:CG	1:A:40:ALA:H	2.17	0.47
1:A:566:ALA:HB1	1:A:578:VAL:HB	1.96	0.47
1:D:318:ASP:HB3	1:D:323:THR:CB	2.40	0.47
1:A:416:HIS:CE1	1:A:418:GLY:HA2	2.49	0.47
1:A:404:LEU:HD21	1:A:511:LEU:HD13	1.97	0.47
1:A:620:VAL:O	1:A:621:THR:CB	2.60	0.46
1:D:263:PRO:HB2	1:D:266:LEU:HG	1.96	0.46
1:A:499:ILE:HG23	1:A:500:ARG:HE	1.79	0.46
1:A:556:ASP:OD1	1:A:557:LYS:HE2	2.15	0.46
1:A:540:MSE:HE3	1:A:543:ARG:HH22	1.80	0.46
1:B:66:SER:HB3	1:B:71:GLU:HG2	1.96	0.46
1:C:157:HIS:HE1	1:C:372:GLY:HA3	1.80	0.46
1:D:164:THR:HG21	1:D:544:ASP:HB2	1.98	0.46
1:A:107:LYS:HE3	3:A:1030:HOH:O	2.14	0.46
1:A:416:HIS:O	1:A:485:PHE:HB2	2.16	0.46
1:C:550:TYR:OH	1:C:583:ASN:O	2.24	0.46
1:D:132:MSE:HE2	1:D:143:PHE:HD2	1.79	0.46
1:D:164:THR:CG2	1:D:544:ASP:HB2	2.45	0.46
1:C:232:THR:OG1	1:C:512:LYS:NZ	2.34	0.46
1:D:264:ARG:O	1:D:268:ASP:N	2.40	0.46
1:A:404:LEU:HB2	1:A:413:TYR:OH	2.16	0.46
1:B:19:THR:HG22	1:B:64:ILE:O	2.16	0.46
1:C:257:PHE:CE2	1:C:259:ILE:HD11	2.51	0.46
1:D:132:MSE:HE1	1:D:143:PHE:CD2	2.48	0.46
1:D:217:LEU:HD11	1:D:223:GLN:HB2	1.98	0.46
1:D:23:GLU:OE2	1:D:79:VAL:HG21	2.15	0.46
1:D:349:GLU:HA	1:D:349:GLU:OE1	2.16	0.46
1:D:484:HIS:HE1	1:D:487:LEU:HG	1.80	0.46
1:D:524:GLN:O	1:D:526:GLU:N	2.49	0.46
1:B:558:ALA:HB2	1:B:631:VAL:HG23	1.97	0.46
1:D:548:TRP:HA	1:D:636:ARG:HG2	1.97	0.46
1:A:286:MSE:HE3	1:A:294:ILE:HG12	1.98	0.46
1:A:28:ALA:HB2	1:A:51:MSE:HE1	1.98	0.46
1:C:184:ASP:HA	1:C:187:LEU:HD11	1.97	0.46
1:D:323:THR:HG21	1:D:326:TRP:O	2.16	0.46
1:A:55:MSE:SE	1:A:83:LEU:CD1	3.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:HB2	1:C:95:ASP:H	1.60	0.45
1:D:636:ARG:HD3	1:D:636:ARG:N	2.31	0.45
1:A:376:ASP:OD1	1:A:377:ILE:N	2.48	0.45
1:A:430:LEU:HD22	1:A:471:PHE:CE1	2.42	0.45
1:A:446:LEU:HD21	1:A:483:PRO:HB2	1.97	0.45
1:C:225:ILE:HA	1:C:284:CYS:O	2.16	0.45
1:C:333:ILE:O	1:C:337:VAL:HG23	2.15	0.45
1:C:5:ASN:ND2	1:C:8:LEU:HB3	2.30	0.45
1:B:416:HIS:ND1	1:B:485:PHE:HB2	2.31	0.45
1:C:5:ASN:HD22	1:C:8:LEU:HB3	1.81	0.45
1:A:231:PRO:HA	1:A:271:CYS:SG	2.56	0.45
1:B:68:LYS:HB2	1:B:69:GLU:H	1.50	0.45
1:B:506:ILE:O	1:B:510:LEU:HG	2.17	0.45
1:A:305:ILE:HG22	1:A:306:GLU:H	1.81	0.45
1:C:198:VAL:HG21	1:C:311:LEU:HD11	1.99	0.45
1:C:185:GLU:H	1:C:187:LEU:HG	1.80	0.45
1:C:222:LEU:HD12	1:C:346:ARG:HD2	1.99	0.45
1:C:398:ILE:O	1:C:402:ARG:HG3	2.17	0.45
1:C:438:VAL:CG1	1:C:443:VAL:HG21	2.47	0.45
1:C:533:GLU:OE1	1:C:533:GLU:HA	2.17	0.45
1:A:319:TRP:CH2	1:A:338:ARG:HG3	2.47	0.45
1:B:430:LEU:O	1:B:434:HIS:HD2	2.00	0.45
1:B:235:ILE:O	1:B:509:ARG:NH2	2.47	0.44
1:B:558:ALA:HB1	1:B:630:GLU:HA	1.99	0.44
1:C:5:ASN:O	1:C:9:ALA:HB2	2.17	0.44
1:D:237:GLU:HB2	1:D:509:ARG:CZ	2.46	0.44
1:D:289:SER:HB3	1:D:290:ALA:H	1.56	0.44
1:A:548:TRP:HA	1:A:636:ARG:HG2	2.00	0.44
1:A:633:MSE:HG2	3:A:1012:HOH:O	2.16	0.44
1:C:30:GLU:OE1	1:C:30:GLU:HA	2.17	0.44
1:D:137:LEU:HA	1:D:137:LEU:HD23	1.70	0.44
1:A:238:GLY:O	1:A:239:SER:C	2.55	0.44
1:C:192:LEU:HB3	1:C:195:LEU:HD12	2.00	0.44
1:C:552:ARG:HA	1:C:633:MSE:HE1	2.00	0.44
1:D:524:GLN:C	1:D:526:GLU:N	2.70	0.44
1:A:135:HIS:ND1	1:A:137:LEU:HB2	2.31	0.44
1:A:344:CYS:HB2	1:A:388:ILE:HA	1.98	0.44
1:A:221:LYS:HD3	1:A:289:SER:HB3	1.99	0.44
1:D:263:PRO:HB3	1:D:265:GLU:OE1	2.16	0.44
1:D:369:GLY:HA3	1:D:373:GLU:OE1	2.18	0.44
1:D:33:PHE:HB3	1:D:48:PRO:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLU:O	1:A:322:ASN:CB	2.65	0.44
1:D:522:ARG:HA	1:D:523:PRO:HD3	1.90	0.44
1:B:29:THR:C	1:B:31:LYS:H	2.21	0.44
1:A:295:GLU:C	1:A:297:ASN:H	2.21	0.44
1:C:182:MSE:HE3	1:C:233:ALA:HB3	2.00	0.44
1:D:208:MSE:HB2	1:D:273:LEU:N	2.33	0.44
1:D:579:ARG:NE	3:D:1041:HOH:O	2.48	0.44
1:A:423:ASN:HB3	1:A:471:PHE:CD2	2.53	0.43
1:B:373:GLU:HG3	3:B:1055:HOH:O	2.18	0.43
1:C:42:LYS:HE2	1:C:44:TYR:CE1	2.52	0.43
1:D:32:GLY:O	1:D:48:PRO:HA	2.18	0.43
1:A:157:HIS:CE1	1:A:552:ARG:NH1	2.87	0.43
1:C:308:LYS:HD3	1:C:308:LYS:HA	1.86	0.43
1:D:426:ALA:HB3	1:D:471:PHE:HE2	1.83	0.43
1:B:570:ASP:OD1	1:B:570:ASP:N	2.50	0.43
1:A:279:ARG:O	1:A:281:VAL:HG23	2.18	0.43
1:B:113:ARG:CB	1:B:113:ARG:NH1	2.81	0.43
1:C:550:TYR:CD2	1:C:585:ALA:HB2	2.54	0.43
1:D:114:ALA:HA	1:D:147:LEU:HB2	2.01	0.43
1:D:47:PRO:HA	1:D:48:PRO:HD3	1.87	0.43
1:B:10:GLN:HA	1:B:13:GLN:HG2	2.01	0.43
1:B:502:TYR:O	1:B:505:MSE:HB2	2.19	0.43
1:C:411:GLY:O	1:C:479:THR:HA	2.18	0.43
1:B:385:ALA:HA	1:B:388:ILE:HD12	2.01	0.43
1:D:229:ALA:HB3	1:D:499:ILE:HD11	2.00	0.43
1:D:95:ASP:OD1	1:D:95:ASP:N	2.52	0.43
1:B:275:ALA:H	1:B:310:LYS:HE3	1.83	0.43
1:B:349:GLU:O	1:B:353:ASN:ND2	2.51	0.43
1:C:111:PRO:HD2	1:C:143:PHE:O	2.19	0.43
1:C:191:ASP:OD1	1:C:193:THR:HB	2.19	0.43
1:D:453:ARG:HA	1:D:453:ARG:HD3	1.72	0.43
1:A:35:PHE:HA	1:A:44:TYR:O	2.18	0.43
1:A:99:ILE:HG23	1:A:99:ILE:O	2.18	0.43
1:B:171:GLU:H	1:B:171:GLU:CD	2.22	0.43
1:C:467:ARG:HA	1:C:467:ARG:NE	2.34	0.43
1:A:157:HIS:HD2	1:A:371:LYS:O	2.02	0.43
1:B:137:LEU:HD23	1:B:137:LEU:HA	1.81	0.43
1:B:177:GLY:O	1:B:178:VAL:C	2.57	0.43
1:B:182:MSE:HE1	1:B:189:ARG:HH12	1.84	0.43
1:B:56:HIS:NE2	1:B:105:LEU:HD13	2.34	0.43
1:B:502:TYR:CE2	1:B:506:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:619:LYS:N	1:D:622:ASP:OD2	2.50	0.42
1:C:524:GLN:OE1	1:C:527:ILE:HG13	2.19	0.42
1:D:9:ALA:O	1:D:13:GLN:HB2	2.19	0.42
1:B:363:ASP:O	1:B:379:ALA:HA	2.20	0.42
1:A:217:LEU:HB3	1:A:218:PRO:CD	2.49	0.42
1:C:429:ALA:HA	1:C:432:LYS:HG2	2.02	0.42
1:C:359:LYS:HE2	1:C:359:LYS:HB3	1.73	0.42
1:D:411:GLY:O	1:D:479:THR:HA	2.19	0.42
1:A:160:PRO:O	1:A:545:VAL:HG22	2.20	0.42
1:B:103:HIS:CE1	1:B:105:LEU:HD12	2.30	0.42
1:B:402:ARG:O	1:B:406:ASP:OD2	2.37	0.42
1:B:93:LYS:O	1:B:94:ASN:C	2.57	0.42
1:C:48:PRO:O	1:C:51:MSE:HB2	2.19	0.42
1:A:324:GLY:O	1:A:325:ASP:HB2	2.19	0.42
1:C:5:ASN:CB	1:C:6:PRO:CD	2.97	0.42
1:D:466:SER:OG	1:D:620:VAL:HG21	2.20	0.42
1:B:561:ASP:HB2	1:B:563:ARG:HH21	1.85	0.42
1:D:275:ALA:HB2	1:D:310:LYS:HG3	2.02	0.42
1:B:5:ASN:HB2	1:B:6:PRO:HD2	2.01	0.41
1:C:55:MSE:CE	1:C:143:PHE:CE2	3.01	0.41
1:D:192:LEU:HB3	1:D:195:LEU:HD12	2.02	0.41
1:A:136:PRO:HA	1:A:140:ASP:O	2.20	0.41
1:A:173:GLU:O	1:A:248:ARG:NH2	2.49	0.41
1:A:280:PRO:HA	1:A:304:THR:HG22	2.01	0.41
1:A:55:MSE:HE3	1:A:143:PHE:CE2	2.54	0.41
1:B:59:ARG:HB3	1:B:80:GLU:HB2	2.01	0.41
1:D:408:LEU:HB3	1:D:410:PHE:HD1	1.85	0.41
1:A:257:PHE:HE2	1:A:259:ILE:HD11	1.83	0.41
1:B:212:LEU:HD21	1:B:393:MSE:CE	2.51	0.41
1:D:243:LYS:HG3	1:D:244:ALA:N	2.35	0.41
1:A:336:GLN:HA	1:A:336:GLN:NE2	2.34	0.41
1:D:416:HIS:ND1	1:D:485:PHE:HB2	2.35	0.41
1:A:221:LYS:NZ	1:A:289:SER:HB3	2.35	0.41
1:B:94:ASN:O	1:B:95:ASP:C	2.58	0.41
1:C:111:PRO:HB2	1:C:144:TYR:CD1	2.55	0.41
1:C:288:LEU:HD11	1:C:343:ILE:HG23	2.02	0.41
1:D:228:ILE:HG13	1:D:496:THR:HA	2.01	0.41
1:D:453:ARG:HH11	1:D:453:ARG:HG2	1.85	0.41
1:A:288:LEU:HD23	1:A:294:ILE:HG13	2.03	0.41
1:B:350:TRP:CD1	1:B:354:HIS:HD2	2.38	0.41
1:A:59:ARG:HB3	1:A:80:GLU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:THR:C	1:B:31:LYS:N	2.71	0.41
1:B:200:ILE:HG12	1:B:311:LEU:HD12	2.03	0.41
1:D:169:ASN:HD22	1:D:169:ASN:HA	1.68	0.41
1:D:407:LYS:HG3	1:D:514:VAL:CG1	2.39	0.41
1:D:171:GLU:CD	1:D:534:ARG:HH12	2.23	0.41
1:A:287:THR:H	1:A:294:ILE:HG23	1.85	0.41
1:C:83:LEU:HD13	1:C:86:PHE:CD2	2.56	0.41
1:A:89:LYS:NZ	1:A:125:GLY:O	2.54	0.41
1:B:268:ASP:O	1:B:272:SER:HB3	2.21	0.41
1:B:41:GLN:HA	1:B:41:GLN:OE1	2.19	0.41
1:D:211:ALA:O	1:D:212:LEU:HD23	2.21	0.41
1:D:256:GLY:HA3	1:D:368:LEU:HD12	2.03	0.41
1:D:464:LEU:HD23	1:D:464:LEU:N	2.35	0.41
1:D:90:VAL:CG1	1:D:91:GLN:N	2.84	0.41
1:C:118:LEU:HD12	1:C:118:LEU:HA	1.97	0.41
1:C:5:ASN:N	1:C:5:ASN:HD22	2.19	0.41
1:D:56:HIS:CE1	1:D:105:LEU:HD13	2.56	0.41
1:A:157:HIS:CD2	1:A:371:LYS:O	2.74	0.40
1:D:198:VAL:HG22	1:D:199:THR:H	1.84	0.40
1:D:633:MSE:C	1:D:635:THR:H	2.24	0.40
1:A:288:LEU:CD2	1:A:294:ILE:HG13	2.52	0.40
1:A:46:ILE:HA	1:A:47:PRO:HD3	1.78	0.40
1:A:602:VAL:O	1:A:610:VAL:HA	2.21	0.40
1:A:95:ASP:HB2	3:A:1039:HOH:O	2.21	0.40
1:B:534:ARG:HD3	1:B:534:ARG:HA	1.88	0.40
1:C:229:ALA:C	1:C:231:PRO:HD3	2.41	0.40
1:C:264:ARG:HA	1:C:267:SER:OG	2.21	0.40
1:D:502:TYR:CD1	1:D:505:MSE:HE2	2.55	0.40
1:A:135:HIS:HA	1:A:136:PRO:HD2	1.91	0.40
1:B:498:PRO:HG3	1:B:508:HIS:CE1	2.55	0.40
1:C:282:LEU:HD12	1:C:283:ALA:H	1.87	0.40
1:D:199:THR:HG22	1:D:210:ASP:O	2.21	0.40
1:D:498:PRO:HB2	1:D:505:MSE:HG2	2.03	0.40
1:B:160:PRO:O	1:B:545:VAL:HG22	2.21	0.40
1:D:304:THR:O	1:D:305:ILE:HG12	2.22	0.40
1:A:273:LEU:HD22	1:A:281:VAL:HG22	2.02	0.40
1:A:568:ILE:HD13	1:A:618:TYR:HB3	2.03	0.40
1:B:183:LEU:HD11	1:B:236:ALA:HB2	2.02	0.40
1:B:187:LEU:HD22	1:B:189:ARG:HH21	1.87	0.40
1:B:411:GLY:O	1:B:413:TYR:HD1	2.04	0.40
1:C:55:MSE:CG	1:C:106:LEU:HD22	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:400:ALA:CB	1:C:495:TRP:CD1	3.05	0.40
1:C:539:ARG:HH11	1:C:539:ARG:HG3	1.86	0.40
1:C:55:MSE:HE3	1:C:55:MSE:HB2	1.92	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	632/644 (98%)	546 (86%)	68 (11%)	18 (3%)	5 2
1	B	632/644 (98%)	577 (91%)	47 (7%)	8 (1%)	12 10
1	C	632/644 (98%)	580 (92%)	45 (7%)	7 (1%)	14 13
1	D	632/644 (98%)	557 (88%)	61 (10%)	14 (2%)	6 4
All	All	2528/2576 (98%)	2260 (89%)	221 (9%)	47 (2%)	8 6

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	218	PRO
1	A	274	ARG
1	A	322	ASN
1	A	325	ASP
1	A	437	HIS
1	A	443	VAL
1	B	322	ASN
1	C	297	ASN
1	D	31	LYS
1	D	221	LYS
1	D	289	SER

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Mol	Chain	Res	Type
1	D	433	THR
1	A	115	ALA
1	A	123	LYS
1	A	187	LEU
1	A	621	THR
1	C	42	LYS
1	C	289	SER
1	C	322	ASN
1	D	68	LYS
1	D	219	ASP
1	D	469	ARG
1	D	525	ASP
1	D	621	THR
1	A	190	GLU
1	A	239	SER
1	A	441	GLU
1	B	15	LEU
1	B	192	LEU
1	B	272	SER
1	C	94	ASN
1	C	182	MSE
1	D	237	GLU
1	D	465	ASP
1	A	39	ASP
1	A	193	THR
1	A	296	ASP
1	B	30	GLU
1	D	220	ASP
1	B	94	ASN
1	B	229	ALA
1	C	188	VAL
1	D	6	PRO
1	A	361	ARG
1	B	255	PRO
1	D	388	ILE

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	480/522 (92%)	445 (93%)	35 (7%)	14	14
1	B	505/522 (97%)	485 (96%)	20 (4%)	31	39
1	C	504/522 (97%)	483 (96%)	21 (4%)	30	36
1	D	479/522 (92%)	456 (95%)	23 (5%)	25	30
All	All	1968/2088 (94%)	1869 (95%)	99 (5%)	24	28

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	17	SER
1	A	18	GLN
1	A	19	THR
1	A	29	THR
1	A	45	PHE
1	A	71	GLU
1	A	76	GLU
1	A	91	GLN
1	A	94	ASN
1	A	133	ARG
1	A	167	ARG
1	A	172	LYS
1	A	178	VAL
1	A	187	LEU
1	A	237	GLU
1	A	258	ASN
1	A	285	ARG
1	A	293	THR
1	A	294	ILE
1	A	305	ILE
1	A	314	ASP
1	A	329	GLU
1	A	344	CYS
1	A	357	VAL
1	A	358	PHE
1	A	417	MSE
1	A	444	LEU
1	A	476	GLU
1	A	511	LEU
1	A	531	MSE

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Mol	Chain	Res	Type
1	A	557	LYS
1	A	582	ASP
1	A	613	LYS
1	A	636	ARG
1	B	29	THR
1	B	68	LYS
1	B	70	ARG
1	B	89	LYS
1	B	113	ARG
1	B	144	TYR
1	B	210	ASP
1	B	232	THR
1	B	258	ASN
1	B	288	LEU
1	B	289	SER
1	B	330	SER
1	B	360	ASP
1	B	367	ILE
1	B	405	ARG
1	B	410	PHE
1	B	472	GLN
1	B	496	THR
1	B	634	GLU
1	B	636	ARG
1	C	5	ASN
1	C	10	GLN
1	C	43	SER
1	C	94	ASN
1	C	113	ARG
1	C	124	GLU
1	C	178	VAL
1	C	198	VAL
1	C	208	MSE
1	C	219	ASP
1	C	267	SER
1	C	268	ASP
1	C	317	SER
1	C	346	ARG
1	C	496	THR
1	C	497	SER
1	C	505	MSE
1	C	524	GLN

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Mol	Chain	Res	Type
1	C	567	GLU
1	C	570	ASP
1	C	636	ARG
1	D	7	LEU
1	D	8	LEU
1	D	43	SER
1	D	70	ARG
1	D	72	SER
1	D	74	GLU
1	D	89	LYS
1	D	95	ASP
1	D	123	LYS
1	D	131	GLU
1	D	180	THR
1	D	187	LEU
1	D	202	SER
1	D	232	THR
1	D	261	MSE
1	D	267	SER
1	D	305	ILE
1	D	349	GLU
1	D	354	HIS
1	D	373	GLU
1	D	436	LEU
1	D	453	ARG
1	D	636	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	91	GLN
1	A	94	ASN
1	A	157	HIS
1	A	605	GLN
1	B	354	HIS
1	B	434	HIS
1	B	507	ASN
1	C	5	ASN
1	C	157	HIS
1	C	315	GLN
1	C	353	ASN

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Mol	Chain	Res	Type
1	C	472	GLN
1	C	611	GLN
1	D	169	ASN
1	D	297	ASN
1	D	342	GLN
1	D	437	HIS
1	D	472	GLN
1	D	607	ASN
1	D	611	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	A	622/644 (96%)	0.41	76 (12%) 4 7	31, 57, 80, 89	0
1	B	622/644 (96%)	-0.06	6 (0%) 82 88	33, 54, 74, 84	0
1	C	622/644 (96%)	-0.19	5 (0%) 86 91	41, 53, 72, 84	0
1	D	622/644 (96%)	0.10	27 (4%) 35 47	31, 53, 74, 85	0
All	All	2488/2576 (96%)	0.06	114 (4%) 32 45	31, 54, 76, 89	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	GLY	7.0
1	A	290	ALA	6.0
1	B	324	GLY	5.9
1	A	195	LEU	5.3
1	A	68	LYS	5.2
1	C	5	ASN	4.6
1	D	219	ASP	4.5
1	A	294	ILE	4.4
1	D	411	GLY	4.4
1	D	183	LEU	4.2
1	D	186	GLY	4.2
1	A	196	ASP	4.2
1	A	288	LEU	4.2
1	A	273	LEU	4.2
1	A	421	PRO	4.1
1	A	183	LEU	4.0
1	A	192	LEU	4.0
1	A	241	LEU	4.0
1	A	311	LEU	3.9
1	A	318	ASP	3.9
1	D	33	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	443	VAL	3.8
1	A	410	PHE	3.7
1	A	187	LEU	3.7
1	C	324	GLY	3.7
1	D	222	LEU	3.7
1	D	421	PRO	3.6
1	A	216	ALA	3.6
1	A	350	TRP	3.5
1	A	407	LYS	3.4
1	A	178	VAL	3.4
1	A	354	HIS	3.4
1	A	295	GLU	3.4
1	D	35	PHE	3.3
1	D	527	ILE	3.3
1	C	41	GLN	3.3
1	A	221	LYS	3.3
1	A	222	LEU	3.3
1	A	296	ASP	3.3
1	A	510	LEU	3.2
1	A	198	VAL	3.1
1	A	474	PHE	3.1
1	A	194	ALA	3.1
1	A	338	ARG	3.1
1	D	32	GLY	3.1
1	A	319	TRP	3.1
1	D	514	VAL	3.0
1	A	287	THR	3.0
1	A	436	LEU	3.0
1	A	514	VAL	3.0
1	A	180	THR	3.0
1	A	278	VAL	3.0
1	A	270	LEU	3.0
1	A	224	LEU	2.9
1	A	358	PHE	2.9
1	A	333	ILE	2.9
1	D	288	LEU	2.9
1	A	302	ALA	2.9
1	A	334	ALA	2.8
1	A	308	LYS	2.8
1	A	213	PHE	2.7
1	A	327	GLN	2.7
1	B	323	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	344	CYS	2.7
1	B	270	LEU	2.7
1	A	186	GLY	2.7
1	A	527	ILE	2.7
1	A	200	ILE	2.6
1	D	5	ASN	2.6
1	A	220	ASP	2.6
1	D	510	LEU	2.6
1	A	197	PHE	2.6
1	A	217	LEU	2.5
1	A	516	LYS	2.5
1	C	185	GLU	2.5
1	A	481	PRO	2.5
1	D	294	ILE	2.5
1	A	329	GLU	2.5
1	A	35	PHE	2.5
1	D	427	LEU	2.5
1	D	410	PHE	2.4
1	D	298	ILE	2.4
1	D	301	PHE	2.4
1	A	185	GLU	2.4
1	A	177	GLY	2.3
1	A	411	GLY	2.3
1	A	72	SER	2.3
1	D	188	VAL	2.3
1	D	322	ASN	2.3
1	A	332	ALA	2.3
1	D	29	THR	2.3
1	A	471	PHE	2.2
1	D	436	LEU	2.2
1	D	334	ALA	2.2
1	D	30	GLU	2.2
1	A	355	ALA	2.2
1	A	440	ALA	2.2
1	A	206	GLU	2.1
1	A	298	ILE	2.1
1	D	324	GLY	2.1
1	C	203	ALA	2.1
1	A	281	VAL	2.1
1	B	300	PHE	2.1
1	A	323	THR	2.1
1	A	301	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	33	PHE	2.1
1	A	431	LEU	2.0
1	A	66	SER	2.0
1	A	455	GLU	2.0
1	A	388	ILE	2.0
1	A	420	ASP	2.0
1	A	276	ASN	2.0
1	D	430	LEU	2.0
1	B	275	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
2	MN	A	1001	1/1	0.85	0.09	100,100,100,100	0
2	MN	C	1003	1/1	0.95	0.03	88,88,88,88	0
2	MN	B	1002	1/1	0.98	0.02	83,83,83,83	0
2	MN	D	1004	1/1	0.99	0.04	94,94,94,94	0

6.5 Other polymers (i)

There are no such residues in this entry.