Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:08 AM GMT

PDB ID	:	2FRX
Title	:	Crystal structure of YebU, a m5C RNA methyltransferase from E.coli
Authors	:	Erlandsen, H.; Nordlund, P.; Hallberg, B.M.; Johnson, K.A.; Ericsson, U.B.
Deposited on	:	2006-01-20
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/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:

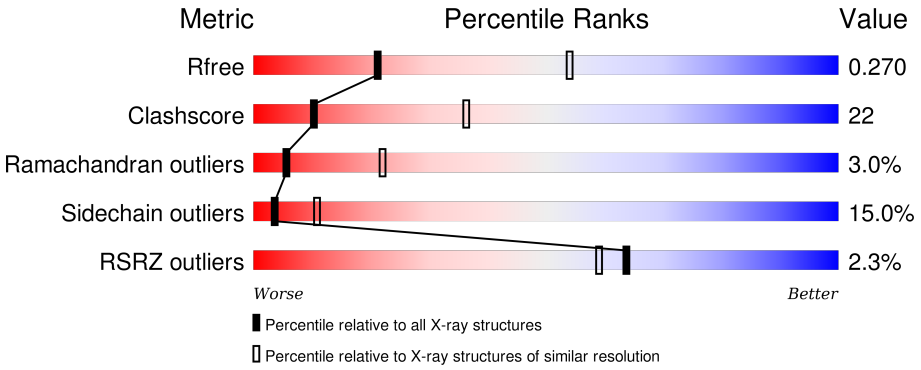
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	479	2% 54% 32% 9% 5%
1	B	479	% 54% 32% 8% 5%
1	C	479	3% 50% 36% 8% • 5%
1	D	479	3% 51% 35% 8% • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14266 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 Hypothetical protein yebU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	Se	0	0	0
			3574	2285	621	654	7	7			
1	B	454	Total	C	N	O	S	Se	0	0	0
			3562	2276	620	652	7	7			
1	C	454	Total	C	N	O	S	Se	0	0	0
			3562	2276	620	652	7	7			
1	D	455	Total	C	N	O	S	Se	0	0	0
			3568	2282	618	654	7	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P76273
A	16	MSE	MET	MODIFIED RESIDUE	UNP P76273
A	20	MSE	MET	MODIFIED RESIDUE	UNP P76273
A	105	MSE	MET	MODIFIED RESIDUE	UNP P76273
A	122	MSE	MET	MODIFIED RESIDUE	UNP P76273
A	139	MSE	MET	MODIFIED RESIDUE	UNP P76273
A	187	MSE	MET	MODIFIED RESIDUE	UNP P76273
A	411	MSE	MET	MODIFIED RESIDUE	UNP P76273
B	1	MSE	MET	MODIFIED RESIDUE	UNP P76273
B	16	MSE	MET	MODIFIED RESIDUE	UNP P76273
B	20	MSE	MET	MODIFIED RESIDUE	UNP P76273
B	105	MSE	MET	MODIFIED RESIDUE	UNP P76273
B	122	MSE	MET	MODIFIED RESIDUE	UNP P76273
B	139	MSE	MET	MODIFIED RESIDUE	UNP P76273
B	187	MSE	MET	MODIFIED RESIDUE	UNP P76273
B	411	MSE	MET	MODIFIED RESIDUE	UNP P76273
C	1	MSE	MET	MODIFIED RESIDUE	UNP P76273
C	16	MSE	MET	MODIFIED RESIDUE	UNP P76273
C	20	MSE	MET	MODIFIED RESIDUE	UNP P76273
C	105	MSE	MET	MODIFIED RESIDUE	UNP P76273
C	122	MSE	MET	MODIFIED RESIDUE	UNP P76273

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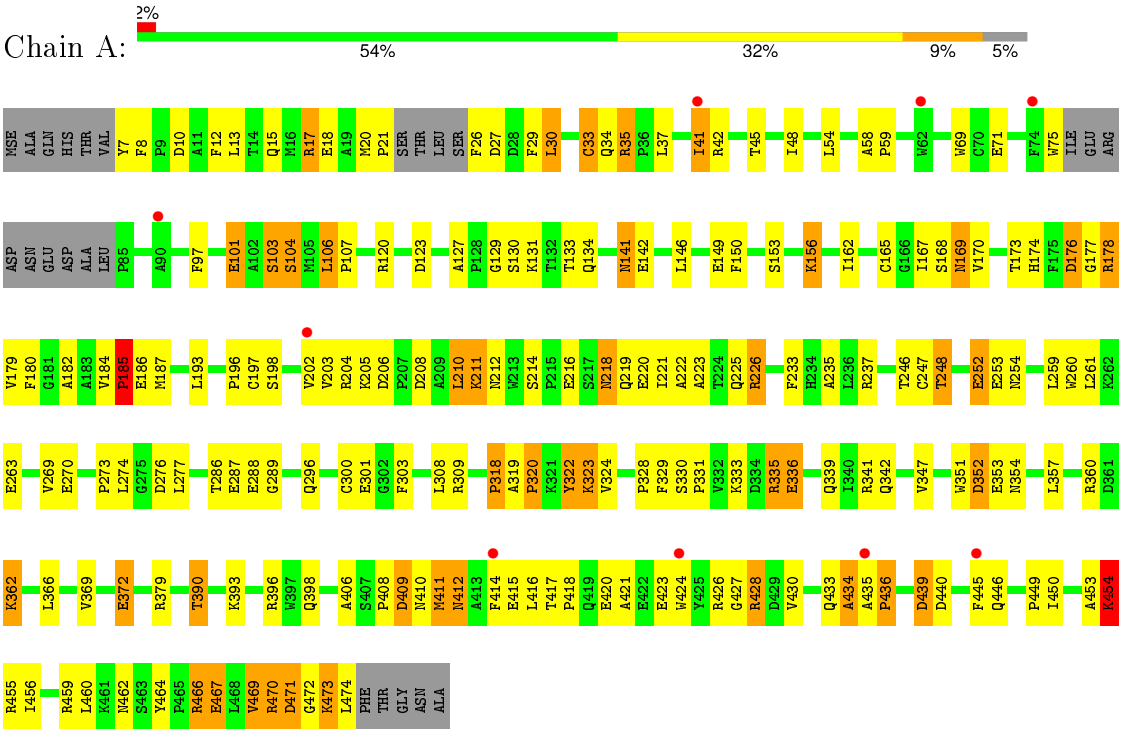
Chain	Residue	Modelled	Actual	Comment	Reference
C	139	MSE	MET	MODIFIED RESIDUE	UNP P76273
C	187	MSE	MET	MODIFIED RESIDUE	UNP P76273
C	411	MSE	MET	MODIFIED RESIDUE	UNP P76273
D	1	MSE	MET	MODIFIED RESIDUE	UNP P76273
D	16	MSE	MET	MODIFIED RESIDUE	UNP P76273
D	20	MSE	MET	MODIFIED RESIDUE	UNP P76273
D	105	MSE	MET	MODIFIED RESIDUE	UNP P76273
D	122	MSE	MET	MODIFIED RESIDUE	UNP P76273
D	139	MSE	MET	MODIFIED RESIDUE	UNP P76273
D	187	MSE	MET	MODIFIED RESIDUE	UNP P76273
D	411	MSE	MET	MODIFIED RESIDUE	UNP P76273

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

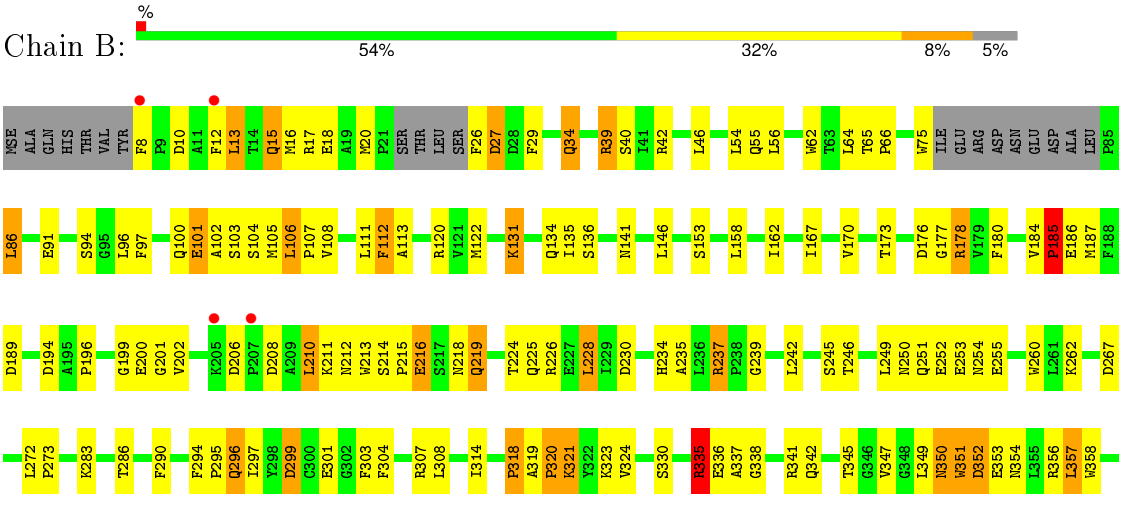
- Molecule 1: Hypothetical protein yebU

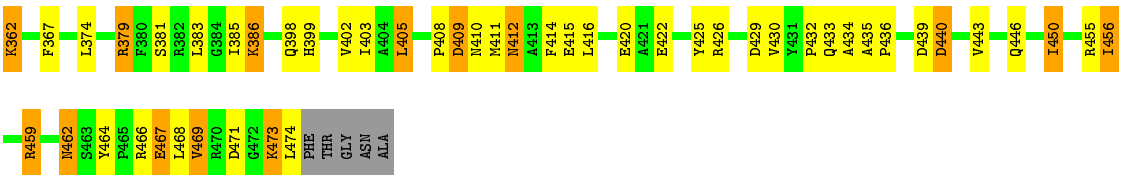
Chain A:



- Molecule 1: Hypothetical protein yebU

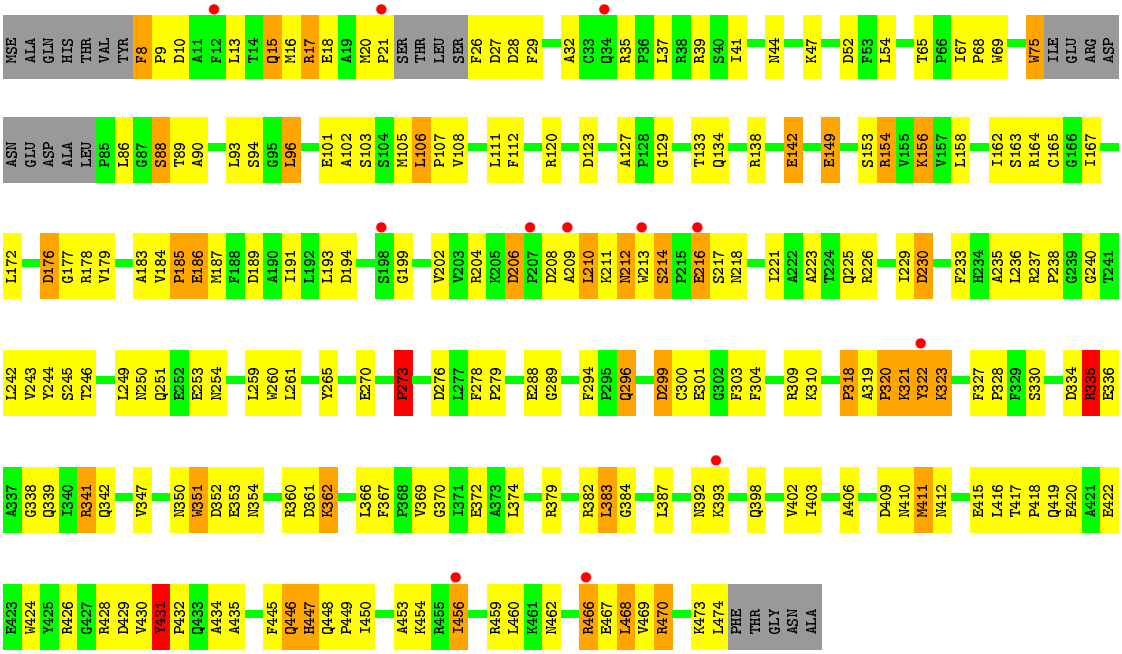
Chain B:





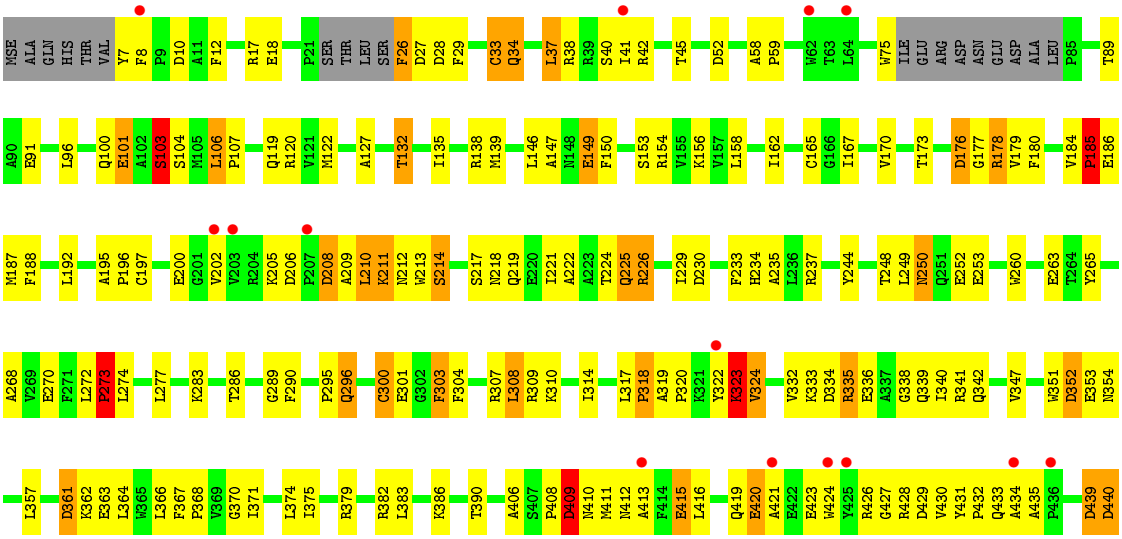
• Molecule 1: Hypothetical protein yebU

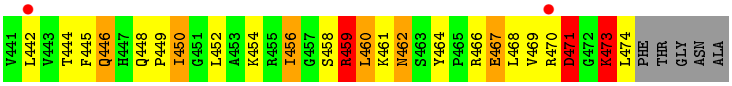
Chain C:



• Molecule 1: Hypothetical protein yebU

Chain D:




V441
L442
V443
T444
F445
Q446
H447
Q448
P449
T450
G451
L452
A453
K454
R455
T456
G457
S458
R459
L460
K461
N462
S463
Y464
P465
R466
E467
L468
V469
R470
D471
G472
K473
L474
PHE
THR
GLY
ASN
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.71Å 87.13Å 95.05Å 88.33° 76.79° 90.19°	Depositor
Resolution (Å)	29.03 – 2.90 29.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.03-2.90) 92.4 (29.03-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.231 , 0.282 0.216 , 0.270	Depositor DCC
R_{free} test set	2314 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	67.5	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 66.4	EDS
Estimated twinning fraction	0.093 for -h,k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 45750 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14266	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.90	12/3659 (0.3%)	0.97	11/4963 (0.2%)
1	B	0.88	4/3646 (0.1%)	0.98	14/4945 (0.3%)
1	C	1.14	13/3646 (0.4%)	1.16	21/4945 (0.4%)
1	D	1.59	38/3653 (1.0%)	1.17	24/4956 (0.5%)
All	All	1.16	67/14604 (0.5%)	1.07	70/19809 (0.4%)

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
1	B	0	2
1	C	0	1
1	D	0	2
All	All	0	6

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	335	ARG	NE-CZ	39.64	1.84	1.33
1	D	420	GLU	CD-OE1	38.71	1.68	1.25
1	C	214	SER	CB-OG	33.06	1.85	1.42
1	D	459	ARG	NE-CZ	22.04	1.61	1.33
1	C	428	ARG	CZ-NH1	20.99	1.60	1.33
1	D	431	TYR	CE1-CZ	18.62	1.62	1.38
1	D	420	GLU	CD-OE2	18.05	1.45	1.25
1	D	10	ASP	CG-OD2	16.12	1.62	1.25
1	D	428	ARG	CZ-NH1	14.25	1.51	1.33
1	D	10	ASP	CG-OD1	13.42	1.56	1.25
1	D	17	ARG	NE-CZ	13.38	1.50	1.33
1	C	17	ARG	CZ-NH1	12.28	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	431	TYR	CG-CD2	12.11	1.54	1.39
1	A	454	LYS	CE-NZ	11.94	1.78	1.49
1	D	431	TYR	CG-CD1	11.90	1.54	1.39
1	C	428	ARG	CZ-NH2	11.69	1.48	1.33
1	D	17	ARG	CD-NE	11.09	1.65	1.46
1	D	428	ARG	NE-CZ	10.94	1.47	1.33
1	D	18	GLU	CD-OE1	10.62	1.37	1.25
1	C	216	GLU	CD-OE2	10.60	1.37	1.25
1	C	428	ARG	CD-NE	10.26	1.63	1.46
1	C	216	GLU	CD-OE1	10.17	1.36	1.25
1	D	18	GLU	CD-OE2	9.83	1.36	1.25
1	D	214	SER	CB-OG	9.72	1.54	1.42
1	C	428	ARG	NE-CZ	9.63	1.45	1.33
1	D	208	ASP	CG-OD1	9.17	1.46	1.25
1	D	17	ARG	CZ-NH1	9.07	1.44	1.33
1	B	18	GLU	CD-OE1	8.81	1.35	1.25
1	A	335	ARG	NE-CZ	8.80	1.44	1.33
1	D	17	ARG	CZ-NH2	-8.59	1.21	1.33
1	D	459	ARG	CG-CD	8.57	1.73	1.51
1	D	208	ASP	CG-OD2	8.24	1.44	1.25
1	D	26	PHE	CG-CD2	7.96	1.50	1.38
1	D	473	LYS	CE-NZ	7.95	1.69	1.49
1	A	18	GLU	CD-OE1	7.69	1.34	1.25
1	D	458	SER	CB-OG	7.69	1.52	1.42
1	A	454	LYS	CD-CE	7.47	1.70	1.51
1	D	283	LYS	CD-CE	7.46	1.69	1.51
1	A	17	ARG	NE-CZ	7.17	1.42	1.33
1	D	339	GLN	CD-OE1	7.13	1.39	1.24
1	D	428	ARG	CZ-NH2	7.05	1.42	1.33
1	D	439	ASP	CG-OD1	7.01	1.41	1.25
1	D	26	PHE	CG-CD1	6.86	1.49	1.38
1	A	27	ASP	CG-OD2	6.75	1.40	1.25
1	A	10	ASP	CG-OD2	6.57	1.40	1.25
1	A	27	ASP	CG-OD1	6.50	1.40	1.25
1	A	428	ARG	CZ-NH1	6.42	1.41	1.33
1	B	34	GLN	CD-OE1	6.37	1.38	1.24
1	D	26	PHE	CE1-CZ	6.28	1.49	1.37
1	D	433	GLN	CD-OE1	6.25	1.37	1.24
1	D	333	LYS	CE-NZ	6.23	1.64	1.49
1	D	26	PHE	CE2-CZ	6.21	1.49	1.37
1	B	18	GLU	CD-OE2	6.20	1.32	1.25
1	C	217	SER	CB-OG	6.12	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CG-CD	6.08	1.61	1.51
1	D	28	ASP	CG-OD2	6.05	1.39	1.25
1	D	423	GLU	CD-OE1	5.95	1.32	1.25
1	D	428	ARG	CG-CD	5.93	1.66	1.51
1	D	335	ARG	CZ-NH2	5.58	1.40	1.33
1	A	71	GLU	CD-OE2	5.56	1.31	1.25
1	C	431	TYR	CG-CD1	5.39	1.46	1.39
1	C	428	ARG	CG-CD	5.29	1.65	1.51
1	C	431	TYR	CE2-CZ	5.20	1.45	1.38
1	A	10	ASP	CG-OD1	5.10	1.37	1.25
1	C	431	TYR	CG-CD2	5.05	1.45	1.39
1	D	431	TYR	CE2-CZ	5.04	1.45	1.38
1	B	10	ASP	CG-OD1	5.03	1.36	1.25

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	428	ARG	NE-CZ-NH2	-30.98	104.81	120.30
1	C	428	ARG	NE-CZ-NH1	30.08	135.34	120.30
1	D	17	ARG	NE-CZ-NH2	22.80	131.70	120.30
1	D	459	ARG	NE-CZ-NH2	-19.50	110.55	120.30
1	D	335	ARG	NE-CZ-NH2	-19.42	110.59	120.30
1	D	428	ARG	NE-CZ-NH2	-17.71	111.44	120.30
1	A	17	ARG	NE-CZ-NH1	13.70	127.15	120.30
1	D	428	ARG	NE-CZ-NH1	11.95	126.28	120.30
1	D	335	ARG	NE-CZ-NH1	11.91	126.25	120.30
1	C	428	ARG	CD-NE-CZ	-10.66	108.68	123.60
1	D	431	TYR	CB-CG-CD1	-9.94	115.04	121.00
1	D	420	GLU	OE1-CD-OE2	9.28	134.43	123.30
1	B	429	ASP	CB-CG-OD2	8.86	126.28	118.30
1	D	471	ASP	CB-CG-OD2	8.45	125.90	118.30
1	D	17	ARG	NH1-CZ-NH2	-8.39	110.17	119.40
1	C	52	ASP	CB-CG-OD2	7.81	125.33	118.30
1	C	206	ASP	CB-CG-OD2	7.63	125.17	118.30
1	D	409	ASP	CB-CG-OD2	7.42	124.97	118.30
1	B	230	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	454	LYS	CD-CE-NZ	-7.23	95.07	111.70
1	A	208	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	276	ASP	CB-CG-OD2	7.16	124.75	118.30
1	C	189	ASP	CB-CG-OD2	7.14	124.73	118.30
1	D	420	GLU	CG-CD-OE1	-7.00	104.31	118.30
1	D	230	ASP	CB-CG-OD2	6.89	124.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	230	ASP	CB-CG-OD2	6.79	124.41	118.30
1	D	431	TYR	CZ-CE2-CD2	-6.75	113.72	119.80
1	C	28	ASP	CB-CG-OD2	6.68	124.31	118.30
1	C	334	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	352	ASP	CB-CA-C	-6.58	97.23	110.40
1	A	30	LEU	CA-CB-CG	6.58	130.43	115.30
1	C	138	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	106	LEU	CA-CB-CG	6.42	130.06	115.30
1	A	206	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	208	ASP	CB-CG-OD2	6.38	124.04	118.30
1	C	123	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	428	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	C	164	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	D	103	SER	N-CA-CB	-6.12	101.31	110.50
1	C	10	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	299	ASP	CB-CG-OD2	6.08	123.78	118.30
1	C	429	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	39	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	B	439	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	374	LEU	CA-CB-CG	5.94	128.97	115.30
1	B	106	LEU	CB-CG-CD2	-5.92	100.93	111.00
1	D	10	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	C	176	ASP	CB-CG-OD2	5.73	123.45	118.30
1	C	27	ASP	CB-CG-OD2	5.69	123.42	118.30
1	C	335	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	27	ASP	CB-CG-OD2	5.55	123.30	118.30
1	B	208	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	334	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	206	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	471	ASP	CB-CG-OD2	5.38	123.14	118.30
1	D	460	LEU	CA-CB-CG	5.33	127.55	115.30
1	B	267	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	352	ASP	CB-CG-OD1	-5.29	113.53	118.30
1	C	194	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	123	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	352	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	52	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	361	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	335	ARG	CG-CD-NE	5.21	122.74	111.80
1	D	440	ASP	CB-CG-OD2	5.17	122.95	118.30
1	D	431	TYR	CB-CG-CD2	5.16	124.10	121.00
1	B	440	ASP	CB-CG-OD2	5.15	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	276	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	120	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	D	308	LEU	CA-CB-CG	5.06	126.93	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	PRO	Peptide
1	B	318	PRO	Peptide
1	B	323	LYS	Peptide
1	C	318	PRO	Peptide
1	D	318	PRO	Peptide
1	D	459	ARG	Sidechain

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	3574	0	3513	132	0
1	B	3562	0	3504	150	0
1	C	3562	0	3504	160	0
1	D	3568	0	3502	171	0
All	All	14266	0	14023	611	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 22.

All (611) 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:473:LYS:NZ	1:D:473:LYS:CE	1.68	1.54
1:A:187:MSE:SE	1:A:187:MSE:CE	2.15	1.45
1:A:411:MSE:SE	1:A:411:MSE:CE	2.14	1.45
1:A:454:LYS:NZ	1:A:454:LYS:CE	1.78	1.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:MSE:CE	1:C:187:MSE:SE	2.17	1.42
1:B:187:MSE:CE	1:B:187:MSE:SE	2.17	1.42
1:D:187:MSE:CE	1:D:187:MSE:SE	2.19	1.39
1:D:335:ARG:NE	1:D:335:ARG:CZ	1.84	1.38
1:C:411:MSE:SE	1:C:411:MSE:CE	2.23	1.36
1:B:411:MSE:SE	1:B:411:MSE:CE	2.21	1.35
1:D:420:GLU:CD	1:D:420:GLU:OE1	1.68	1.29
1:B:318:PRO:O	1:B:320:PRO:HD3	1.33	1.28
1:D:318:PRO:O	1:D:320:PRO:HD3	1.31	1.27
1:C:214:SER:OG	1:C:214:SER:CB	1.85	1.24
1:C:318:PRO:O	1:C:320:PRO:HD3	1.35	1.21
1:B:94:SER:HB3	1:B:450:ILE:HD11	1.28	1.14
1:C:29:PHE:HA	1:C:296:GLN:HG2	1.30	1.12
1:B:341:ARG:HG2	1:B:351:TRP:HZ2	1.01	1.09
1:B:122:MSE:HE1	1:B:180:PHE:CE2	1.88	1.09
1:B:341:ARG:HG2	1:B:351:TRP:CZ2	1.90	1.06
1:B:335:ARG:HH11	1:B:335:ARG:CG	1.72	1.02
1:B:335:ARG:HG3	1:B:335:ARG:NH1	1.62	1.02
1:C:335:ARG:HB3	1:C:335:ARG:HH11	1.20	1.00
1:A:318:PRO:O	1:A:320:PRO:HD3	1.59	1.00
1:A:223:ALA:HA	1:A:226:ARG:NH1	1.78	0.97
1:C:108:VAL:HG11	1:C:134:GLN:HG2	1.46	0.96
1:B:94:SER:HB3	1:B:450:ILE:CD1	1.95	0.96
1:B:416:LEU:HD22	1:B:420:GLU:HB3	1.47	0.96
1:B:341:ARG:CG	1:B:351:TRP:HZ2	1.78	0.96
1:D:106:LEU:HB3	1:D:107:PRO:HD3	1.48	0.95
1:B:225:GLN:HE22	1:B:253:GLU:HB3	1.32	0.95
1:C:341:ARG:HD3	1:C:351:TRP:CH2	2.02	0.94
1:B:29:PHE:HA	1:B:296:GLN:HG2	1.47	0.94
1:B:335:ARG:HH11	1:B:335:ARG:HG3	0.81	0.94
1:D:318:PRO:O	1:D:320:PRO:CD	2.17	0.92
1:A:225:GLN:OE1	1:A:253:GLU:HG2	1.71	0.91
1:B:399:HIS:CE1	1:B:403:ILE:HD11	2.06	0.91
1:C:176:ASP:O	1:C:178:ARG:N	2.06	0.88
1:C:318:PRO:O	1:C:320:PRO:CD	2.21	0.88
1:C:352:ASP:HB3	1:C:354:ASN:H	1.39	0.88
1:C:236:LEU:HD11	1:C:240:GLY:HA3	1.56	0.87
1:A:352:ASP:HB3	1:A:354:ASN:H	1.40	0.86
1:D:226:ARG:HG3	1:D:226:ARG:NH1	1.88	0.86
1:B:425:TYR:OH	1:B:450:ILE:CD1	2.25	0.85
1:A:416:LEU:HD22	1:A:420:GLU:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:MSE:HE3	1:C:21:PRO:HD2	1.59	0.83
1:B:176:ASP:O	1:B:178:ARG:N	2.11	0.83
1:D:318:PRO:C	1:D:320:PRO:HD3	1.98	0.82
1:A:223:ALA:HA	1:A:226:ARG:HH11	1.43	0.82
1:D:176:ASP:O	1:D:178:ARG:N	2.13	0.82
1:B:318:PRO:O	1:B:320:PRO:CD	2.25	0.81
1:D:226:ARG:HH11	1:D:226:ARG:HG3	1.42	0.81
1:D:103:SER:HB2	1:D:301:GLU:OE2	1.81	0.81
1:D:324:VAL:HG12	1:D:379:ARG:HE	1.43	0.81
1:B:184:VAL:HG12	1:B:187:MSE:HB2	1.60	0.81
1:D:185:PRO:O	1:D:235:ALA:HA	1.81	0.81
1:B:131:LYS:O	1:B:135:ILE:HG12	1.79	0.81
1:B:16:MSE:HE1	1:B:249:LEU:HB2	1.63	0.80
1:C:341:ARG:HD3	1:C:351:TRP:HH2	1.45	0.80
1:C:210:LEU:O	1:C:212:ASN:N	2.15	0.80
1:C:223:ALA:HA	1:C:226:ARG:HH12	1.47	0.80
1:D:363:GLU:HG2	1:D:386:LYS:HE3	1.64	0.79
1:A:176:ASP:O	1:A:178:ARG:N	2.16	0.79
1:A:185:PRO:O	1:A:235:ALA:HA	1.83	0.79
1:B:367:PHE:CE1	1:B:383:LEU:HB2	2.17	0.79
1:A:410:ASN:OD1	1:A:412:ASN:N	2.16	0.78
1:A:318:PRO:C	1:A:320:PRO:HD3	2.02	0.78
1:C:185:PRO:O	1:C:235:ALA:HA	1.83	0.77
1:B:352:ASP:HB2	1:B:354:ASN:H	1.49	0.77
1:D:178:ARG:HH11	1:D:178:ARG:HG3	1.46	0.77
1:C:127:ALA:HB1	1:C:154:ARG:HG2	1.67	0.77
1:B:219:GLN:OE1	1:B:219:GLN:HA	1.84	0.77
1:D:122:MSE:CE	1:D:146:LEU:HD22	2.15	0.77
1:A:29:PHE:HA	1:A:296:GLN:HG2	1.66	0.77
1:C:26:PHE:O	1:C:29:PHE:HB3	1.84	0.76
1:D:351:TRP:HE3	1:D:352:ASP:O	1.67	0.76
1:A:221:ILE:O	1:A:225:GLN:HG3	1.86	0.76
1:D:429:ASP:OD1	1:D:461:LYS:HA	1.86	0.75
1:B:122:MSE:HE1	1:B:180:PHE:CZ	2.21	0.75
1:B:351:TRP:HE3	1:B:351:TRP:O	1.69	0.75
1:C:223:ALA:HA	1:C:226:ARG:NH1	2.02	0.75
1:B:466:ARG:HA	1:B:469:VAL:HG13	1.67	0.75
1:D:416:LEU:HD22	1:D:420:GLU:HB3	1.67	0.75
1:C:318:PRO:C	1:C:320:PRO:HD3	2.06	0.75
1:D:341:ARG:CG	1:D:351:TRP:HZ2	2.01	0.74
1:A:445:PHE:HB3	1:A:450:ILE:CD1	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:PRO:C	1:B:320:PRO:HD3	2.07	0.74
1:B:341:ARG:NH2	1:B:351:TRP:CH2	2.56	0.74
1:A:103:SER:HB2	1:A:301:GLU:OE1	1.87	0.74
1:A:219:GLN:HA	1:A:219:GLN:OE1	1.85	0.74
1:D:226:ARG:HH11	1:D:226:ARG:CG	2.01	0.73
1:C:246:THR:OG1	1:C:254:ASN:ND2	2.20	0.73
1:C:341:ARG:HB2	1:C:351:TRP:CZ2	2.24	0.73
1:B:362:LYS:HD3	1:B:362:LYS:N	2.04	0.73
1:D:127:ALA:HB2	1:D:149:GLU:HG3	1.70	0.73
1:A:197:CYS:HB2	1:A:248:THR:CG2	2.19	0.73
1:C:335:ARG:HH11	1:C:335:ARG:CB	2.01	0.73
1:A:176:ASP:OD1	1:A:176:ASP:N	2.22	0.73
1:D:341:ARG:HG2	1:D:351:TRP:CZ2	2.23	0.72
1:D:153:SER:HA	1:D:156:LYS:HE3	1.71	0.72
1:D:225:GLN:HE22	1:D:253:GLU:HG2	1.54	0.72
1:B:26:PHE:O	1:B:29:PHE:HB3	1.89	0.72
1:D:270:GLU:OE1	1:D:309:ARG:NH1	2.22	0.72
1:B:425:TYR:OH	1:B:450:ILE:HD13	1.90	0.72
1:D:150:PHE:CE2	1:D:176:ASP:HB3	2.25	0.72
1:D:29:PHE:HA	1:D:296:GLN:CG	2.19	0.72
1:B:210:LEU:O	1:B:212:ASN:N	2.22	0.71
1:C:367:PHE:CE1	1:C:383:LEU:HB2	2.25	0.71
1:B:108:VAL:HG11	1:B:134:GLN:HG2	1.73	0.71
1:C:338:GLY:HA2	1:C:341:ARG:NH2	2.06	0.71
1:A:473:LYS:H	1:A:473:LYS:NZ	1.89	0.71
1:D:106:LEU:HB3	1:D:107:PRO:CD	2.19	0.70
1:D:150:PHE:HE2	1:D:176:ASP:HB3	1.55	0.70
1:C:29:PHE:HB2	1:C:296:GLN:NE2	2.06	0.69
1:D:357:LEU:HG	1:D:366:LEU:HD23	1.74	0.69
1:C:369:VAL:HA	1:C:372:GLU:OE2	1.92	0.69
1:C:158:LEU:HD22	1:C:172:LEU:HD21	1.75	0.69
1:A:198:SER:HB3	1:A:218:ASN:HD21	1.57	0.69
1:A:7:TYR:CD2	1:A:211:LYS:HD2	2.28	0.69
1:C:16:MSE:HE1	1:C:249:LEU:HB2	1.75	0.68
1:D:210:LEU:O	1:D:212:ASN:N	2.26	0.68
1:A:196:PRO:O	1:A:225:GLN:NE2	2.27	0.68
1:A:165:CYS:HB2	1:A:167:ILE:HD12	1.74	0.68
1:C:29:PHE:CA	1:C:296:GLN:HG2	2.18	0.68
1:D:29:PHE:HA	1:D:296:GLN:HG2	1.75	0.68
1:D:165:CYS:HB2	1:D:167:ILE:HD12	1.75	0.68
1:B:324:VAL:HG12	1:B:324:VAL:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:THR:HG22	1:B:228:LEU:HD12	1.74	0.68
1:C:236:LEU:O	1:C:310:LYS:HE3	1.92	0.68
1:A:274:LEU:HD22	1:A:277:LEU:HD22	1.76	0.67
1:A:454:LYS:NZ	1:A:454:LYS:CD	2.57	0.67
1:B:176:ASP:CG	1:B:176:ASP:O	2.32	0.67
1:B:399:HIS:CE1	1:B:403:ILE:CD1	2.77	0.67
1:C:127:ALA:HB2	1:C:149:GLU:HG3	1.74	0.67
1:A:210:LEU:O	1:A:212:ASN:N	2.28	0.67
1:C:106:LEU:HB3	1:C:107:PRO:HD3	1.76	0.67
1:A:45:THR:HG22	1:A:45:THR:O	1.93	0.67
1:A:445:PHE:HB3	1:A:450:ILE:HD12	1.77	0.67
1:C:172:LEU:HD12	1:C:382:ARG:HB3	1.76	0.67
1:B:242:LEU:HD23	1:B:308:LEU:HD11	1.76	0.67
1:D:127:ALA:HB1	1:D:154:ARG:HG2	1.76	0.67
1:B:102:ALA:HA	1:B:105:MSE:HE3	1.76	0.67
1:B:184:VAL:HG12	1:B:187:MSE:CB	2.25	0.67
1:B:122:MSE:CE	1:B:146:LEU:HD22	2.25	0.67
1:A:197:CYS:HB2	1:A:248:THR:HG21	1.77	0.66
1:A:439:ASP:HB3	1:A:455:ARG:HE	1.61	0.66
1:C:156:LYS:O	1:C:156:LYS:HE2	1.95	0.66
1:D:96:LEU:HD21	1:D:448:GLN:HG3	1.78	0.66
1:C:328:PRO:O	1:C:360:ARG:HG3	1.96	0.66
1:D:178:ARG:HH11	1:D:178:ARG:CG	2.09	0.65
1:B:176:ASP:OD1	1:B:176:ASP:O	2.14	0.65
1:D:226:ARG:O	1:D:229:ILE:HG22	1.96	0.65
1:B:414:PHE:CE2	1:B:436:PRO:HD3	2.30	0.65
1:A:466:ARG:O	1:A:469:VAL:HG12	1.97	0.65
1:D:429:ASP:OD1	1:D:462:ASN:N	2.27	0.65
1:C:230:ASP:OD2	1:C:265:TYR:OH	2.09	0.65
1:B:341:ARG:CG	1:B:351:TRP:CZ2	2.65	0.65
1:A:287:GLU:HG3	1:B:379:ARG:NE	2.11	0.65
1:C:101:GLU:HB3	1:C:301:GLU:OE2	1.95	0.65
1:D:42:ARG:HE	1:D:100:GLN:HE21	1.44	0.64
1:D:448:GLN:O	1:D:450:ILE:HD13	1.97	0.64
1:D:296:GLN:H	1:D:296:GLN:HE21	1.44	0.64
1:D:122:MSE:HE2	1:D:146:LEU:HD22	1.79	0.64
1:D:150:PHE:HD2	1:D:176:ASP:HA	1.62	0.64
1:D:341:ARG:CG	1:D:351:TRP:CZ2	2.79	0.64
1:A:369:VAL:HA	1:A:372:GLU:OE1	1.97	0.64
1:D:357:LEU:HG	1:D:366:LEU:CD2	2.28	0.63
1:D:37:LEU:HD12	1:D:38:ARG:H	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:MSE:HE1	1:B:296:GLN:OE1	1.99	0.63
1:C:191:ILE:HD12	1:C:236:LEU:HB2	1.80	0.63
1:D:219:GLN:HA	1:D:219:GLN:OE1	1.98	0.63
1:D:150:PHE:CD2	1:D:176:ASP:HA	2.32	0.63
1:B:189:ASP:HB2	1:B:237:ARG:NH1	2.14	0.62
1:D:7:TYR:HE2	1:D:211:LYS:HA	1.63	0.62
1:D:351:TRP:CE3	1:D:352:ASP:O	2.51	0.62
1:A:210:LEU:HD12	1:A:211:LYS:N	2.14	0.62
1:A:153:SER:O	1:A:156:LYS:HD3	2.00	0.62
1:C:176:ASP:CG	1:C:176:ASP:O	2.36	0.62
1:D:58:ALA:N	1:D:59:PRO:HD2	2.14	0.62
1:B:122:MSE:HE3	1:B:146:LEU:HD22	1.82	0.62
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.82	0.62
1:D:7:TYR:CE2	1:D:211:LYS:HA	2.35	0.62
1:C:221:ILE:O	1:C:225:GLN:HG3	2.00	0.61
1:C:226:ARG:O	1:C:229:ILE:HG22	2.00	0.61
1:B:351:TRP:CE3	1:B:351:TRP:O	2.52	0.61
1:D:274:LEU:HD22	1:D:277:LEU:HD22	1.81	0.61
1:A:430:VAL:O	1:A:459:ARG:O	2.18	0.61
1:B:338:GLY:HA2	1:B:341:ARG:HD2	1.83	0.61
1:C:142:GLU:OE2	1:C:142:GLU:HA	2.01	0.61
1:A:396:ARG:O	1:A:398:GLN:NE2	2.33	0.60
1:B:324:VAL:CG1	1:B:324:VAL:O	2.49	0.60
1:B:108:VAL:HG13	1:B:135:ILE:HD13	1.84	0.60
1:B:341:ARG:HB3	1:B:351:TRP:CZ2	2.37	0.60
1:B:225:GLN:NE2	1:B:253:GLU:HB3	2.10	0.60
1:C:108:VAL:CG1	1:C:134:GLN:HG2	2.29	0.60
1:A:445:PHE:HB3	1:A:450:ILE:HD11	1.83	0.60
1:C:236:LEU:HD11	1:C:240:GLY:CA	2.30	0.60
1:A:223:ALA:CA	1:A:226:ARG:NH1	2.61	0.59
1:A:29:PHE:CA	1:A:296:GLN:HG2	2.33	0.59
1:A:58:ALA:N	1:A:59:PRO:HD2	2.16	0.59
1:D:127:ALA:H	1:D:149:GLU:HG2	1.66	0.59
1:B:162:ILE:CD1	1:B:170:VAL:HG11	2.33	0.59
1:C:94:SER:HB3	1:C:450:ILE:HD11	1.85	0.59
1:A:318:PRO:O	1:A:320:PRO:CD	2.43	0.59
1:D:26:PHE:O	1:D:29:PHE:HB3	2.01	0.59
1:B:42:ARG:HE	1:B:100:GLN:NE2	2.00	0.59
1:C:16:MSE:HE1	1:C:249:LEU:CB	2.33	0.59
1:C:456:ILE:HG21	1:C:459:ARG:NH2	2.18	0.58
1:D:410:ASN:HD22	1:D:413:ALA:N	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:O	1:A:202:VAL:HG12	2.03	0.58
1:B:42:ARG:HE	1:B:100:GLN:HE21	1.51	0.58
1:D:178:ARG:NH1	1:D:178:ARG:HG3	2.17	0.58
1:C:229:ILE:HG12	1:C:261:LEU:HD22	1.86	0.58
1:B:40:SER:OG	1:B:100:GLN:O	2.20	0.58
1:C:456:ILE:HG21	1:C:459:ARG:HH22	1.69	0.58
1:C:338:GLY:HA2	1:C:341:ARG:HH21	1.68	0.58
1:B:162:ILE:HG23	1:B:167:ILE:HB	1.86	0.58
1:A:445:PHE:CB	1:A:450:ILE:HD12	2.33	0.58
1:D:430:VAL:O	1:D:459:ARG:O	2.22	0.57
1:C:278:PHE:HB2	1:C:279:PRO:HD2	1.86	0.57
1:C:16:MSE:HE3	1:C:29:PHE:CZ	2.39	0.57
1:B:337:ALA:O	1:B:341:ARG:HG3	2.05	0.57
1:A:7:TYR:O	1:A:210:LEU:HD11	2.04	0.57
1:A:45:THR:HA	1:A:48:ILE:O	2.04	0.57
1:A:104:SER:OG	1:A:131:LYS:HE3	2.05	0.57
1:A:473:LYS:H	1:A:473:LYS:HZ3	1.52	0.57
1:B:27:ASP:N	1:B:27:ASP:OD2	2.29	0.57
1:D:221:ILE:O	1:D:224:THR:HB	2.05	0.57
1:B:29:PHE:CA	1:B:296:GLN:HG2	2.29	0.57
1:C:398:GLN:O	1:C:402:VAL:HG23	2.05	0.57
1:A:69:TRP:CG	1:A:106:LEU:HD13	2.40	0.56
1:B:201:GLY:O	1:B:301:GLU:HG2	2.05	0.56
1:D:286:THR:OG1	1:D:290:PHE:HB2	2.04	0.56
1:B:136:SER:HB3	1:B:167:ILE:HD12	1.87	0.56
1:A:357:LEU:HD13	1:A:366:LEU:HD21	1.88	0.56
1:C:129:GLY:O	1:C:133:THR:HG23	2.05	0.56
1:C:29:PHE:HB2	1:C:296:GLN:HE21	1.70	0.56
1:B:352:ASP:CB	1:B:354:ASN:H	2.18	0.56
1:A:197:CYS:HB2	1:A:248:THR:HG22	1.88	0.56
1:B:350:ASN:O	1:B:405:LEU:HB3	2.05	0.56
1:C:47:LYS:NZ	1:C:403:ILE:HG23	2.20	0.56
1:A:141:ASN:HD21	1:A:168:SER:H	1.53	0.56
1:D:250:ASN:ND2	1:D:253:GLU:H	2.04	0.55
1:B:46:LEU:CD1	1:B:167:ILE:HD13	2.35	0.55
1:B:185:PRO:O	1:B:235:ALA:HA	2.06	0.55
1:D:250:ASN:HD21	1:D:253:GLU:H	1.53	0.55
1:B:216:GLU:N	1:B:216:GLU:OE2	2.38	0.55
1:B:349:LEU:HD21	1:B:402:VAL:HA	1.86	0.55
1:C:470:ARG:HG2	1:C:474:LEU:HD21	1.88	0.55
1:C:105:MSE:HA	1:C:134:GLN:HE22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HB3	1:B:307:ARG:HE	1.71	0.55
1:D:37:LEU:HD21	1:D:301:GLU:OE1	2.07	0.55
1:B:430:VAL:O	1:B:459:ARG:O	2.24	0.55
1:C:242:LEU:HD12	1:C:243:VAL:N	2.22	0.55
1:D:132:THR:HG21	1:D:147:ALA:HB2	1.87	0.55
1:B:106:LEU:HB3	1:B:107:PRO:HD3	1.87	0.55
1:C:47:LYS:HZ1	1:C:403:ILE:HG23	1.70	0.55
1:D:222:ALA:O	1:D:226:ARG:HG2	2.07	0.54
1:D:37:LEU:HD21	1:D:301:GLU:HG3	1.87	0.54
1:D:352:ASP:HB3	1:D:354:ASN:H	1.72	0.54
1:A:261:LEU:HD23	1:A:308:LEU:CD2	2.37	0.54
1:B:415:GLU:OE1	1:B:446:GLN:N	2.41	0.54
1:A:415:GLU:OE2	1:A:446:GLN:N	2.39	0.54
1:D:186:GLU:HB3	1:D:237:ARG:HA	1.89	0.54
1:D:272:LEU:HD11	1:D:309:ARG:HB2	1.88	0.54
1:D:127:ALA:HB2	1:D:149:GLU:CG	2.36	0.54
1:A:270:GLU:OE2	1:A:309:ARG:NH2	2.41	0.54
1:B:237:ARG:HH21	1:B:239:GLY:HA3	1.73	0.54
1:D:347:VAL:O	1:D:347:VAL:HG12	2.07	0.54
1:D:103:SER:HB2	1:D:301:GLU:CD	2.27	0.54
1:D:332:VAL:HG13	1:D:336:GLU:OE2	2.07	0.54
1:D:206:ASP:HB3	1:D:209:ALA:HB2	1.89	0.54
1:B:162:ILE:HD13	1:B:170:VAL:HG11	1.89	0.53
1:B:186:GLU:HB3	1:B:237:ARG:HA	1.89	0.53
1:D:192:LEU:HD23	1:D:192:LEU:C	2.28	0.53
1:D:202:VAL:O	1:D:202:VAL:HG12	2.08	0.53
1:B:215:PRO:O	1:B:218:ASN:HB2	2.09	0.53
1:D:410:ASN:ND2	1:D:412:ASN:OD1	2.41	0.53
1:B:113:ALA:HB3	1:B:307:ARG:NH1	2.22	0.53
1:A:406:ALA:HB3	1:A:449:PRO:HB3	1.91	0.53
1:D:233:PHE:CZ	1:D:310:LYS:HG3	2.43	0.53
1:A:129:GLY:O	1:A:133:THR:HG23	2.08	0.53
1:C:8:PHE:CD1	1:C:8:PHE:N	2.74	0.53
1:A:330:SER:OG	1:A:331:PRO:HD2	2.08	0.53
1:D:200:GLU:CD	1:D:249:LEU:H	2.11	0.53
1:C:218:ASN:ND2	1:C:253:GLU:OE2	2.41	0.53
1:D:416:LEU:HD13	1:D:421:ALA:HA	1.90	0.53
1:D:415:GLU:HG2	1:D:444:THR:OG1	2.08	0.53
1:A:12:PHE:CE2	1:A:13:LEU:HD23	2.44	0.53
1:C:335:ARG:NH1	1:C:336:GLU:H	2.07	0.53
1:C:430:VAL:O	1:C:459:ARG:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:VAL:O	1:B:347:VAL:CG1	2.57	0.53
1:B:341:ARG:CB	1:B:351:TRP:CZ2	2.92	0.52
1:B:146:LEU:HD23	1:B:146:LEU:C	2.30	0.52
1:A:424:TRP:HH2	1:A:453:ALA:HB2	1.74	0.52
1:C:29:PHE:HA	1:C:296:GLN:CG	2.20	0.52
1:D:158:LEU:O	1:D:162:ILE:HG13	2.10	0.52
1:D:229:ILE:HD13	1:D:244:TYR:CD2	2.44	0.52
1:D:162:ILE:HG23	1:D:167:ILE:HB	1.90	0.52
1:B:226:ARG:HD2	1:B:260:TRP:CD2	2.45	0.52
1:D:197:CYS:HB2	1:D:253:GLU:OE2	2.09	0.52
1:D:29:PHE:CA	1:D:296:GLN:HG2	2.40	0.52
1:D:466:ARG:HA	1:D:469:VAL:HG13	1.91	0.52
1:D:200:GLU:HG3	1:D:248:THR:HA	1.91	0.52
1:B:356:ARG:HH11	1:B:356:ARG:HG2	1.75	0.52
1:D:208:ASP:O	1:D:211:LYS:HG3	2.09	0.52
1:A:417:THR:HB	1:A:418:PRO:HD2	1.92	0.52
1:D:180:PHE:O	1:D:184:VAL:HG12	2.10	0.52
1:B:17:ARG:NH2	1:B:26:PHE:CE2	2.76	0.52
1:C:165:CYS:HB2	1:C:167:ILE:HD12	1.92	0.52
1:A:269:VAL:CG1	1:A:308:LEU:HD23	2.39	0.51
1:D:29:PHE:HA	1:D:296:GLN:HG3	1.90	0.51
1:A:127:ALA:HB3	1:A:149:GLU:OE2	2.10	0.51
1:A:186:GLU:HB3	1:A:237:ARG:HA	1.92	0.51
1:C:322:TYR:O	1:C:323:LYS:C	2.49	0.51
1:A:210:LEU:HD12	1:A:211:LYS:H	1.76	0.51
1:A:261:LEU:HD23	1:A:308:LEU:HD22	1.91	0.51
1:B:202:VAL:HG12	1:B:202:VAL:O	2.10	0.51
1:D:368:PRO:O	1:D:371:ILE:HG22	2.11	0.51
1:D:341:ARG:HG3	1:D:351:TRP:HZ2	1.75	0.51
1:A:439:ASP:HA	1:A:455:ARG:HB2	1.92	0.51
1:C:245:SER:HA	1:C:304:PHE:O	2.11	0.51
1:C:193:LEU:HD23	1:C:244:TYR:CD2	2.46	0.51
1:D:420:GLU:OE1	1:D:420:GLU:CG	2.55	0.50
1:B:425:TYR:OH	1:B:450:ILE:HD11	2.07	0.50
1:A:184:VAL:HG22	1:A:187:MSE:HB2	1.92	0.50
1:C:102:ALA:HA	1:C:105:MSE:HE3	1.92	0.50
1:D:184:VAL:HG22	1:D:187:MSE:HB2	1.92	0.50
1:D:324:VAL:HG12	1:D:379:ARG:NE	2.21	0.50
1:B:122:MSE:HE1	1:B:180:PHE:CD2	2.42	0.50
1:C:127:ALA:H	1:C:149:GLU:HG2	1.77	0.50
1:D:338:GLY:O	1:D:341:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:TYR:HB3	1:D:268:ALA:HB3	1.93	0.50
1:C:341:ARG:CB	1:C:351:TRP:CZ2	2.92	0.50
1:D:26:PHE:CD2	1:D:26:PHE:C	2.84	0.50
1:A:187:MSE:HB2	1:A:187:MSE:CE	2.42	0.50
1:D:37:LEU:HD12	1:D:38:ARG:N	2.27	0.50
1:A:273:PRO:HA	1:A:289:GLY:HA3	1.94	0.50
1:C:111:LEU:HD12	1:C:243:VAL:HG23	1.93	0.49
1:D:406:ALA:HB3	1:D:449:PRO:HB3	1.94	0.49
1:A:426:ARG:NH2	1:A:472:GLY:O	2.44	0.49
1:D:250:ASN:HD22	1:D:252:GLU:N	2.10	0.49
1:B:224:THR:HG22	1:B:228:LEU:CD1	2.40	0.49
1:D:324:VAL:HA	1:D:379:ARG:HH21	1.76	0.49
1:C:445:PHE:C	1:C:446:GLN:HG2	2.33	0.49
1:C:20:MSE:HE1	1:C:294:PHE:CD1	2.48	0.49
1:A:29:PHE:O	1:A:33:CYS:HB2	2.13	0.49
1:C:101:GLU:CB	1:C:301:GLU:OE2	2.59	0.49
1:C:193:LEU:HD23	1:C:244:TYR:HD2	1.77	0.49
1:D:234:HIS:CE1	1:D:314:ILE:CD1	2.95	0.49
1:C:446:GLN:O	1:C:447:HIS:HB2	2.12	0.49
1:A:470:ARG:HG2	1:A:474:LEU:HD21	1.94	0.49
1:B:294:PHE:HB3	1:B:295:PRO:HD2	1.95	0.49
1:C:288:GLU:OE1	1:C:288:GLU:N	2.45	0.49
1:A:252:GLU:OE2	1:A:252:GLU:N	2.39	0.49
1:D:420:GLU:CB	1:D:420:GLU:OE1	2.61	0.49
1:D:456:ILE:HG21	1:D:459:ARG:HE	1.77	0.49
1:B:186:GLU:O	1:B:237:ARG:HB3	2.11	0.49
1:A:286:THR:HB	1:A:288:GLU:OE2	2.13	0.49
1:C:184:VAL:O	1:C:184:VAL:HG13	2.13	0.49
1:A:252:GLU:H	1:A:252:GLU:CD	2.15	0.49
1:A:414:PHE:CE2	1:A:436:PRO:HD3	2.48	0.49
1:A:424:TRP:CH2	1:A:453:ALA:HB2	2.47	0.49
1:C:309:ARG:HG3	1:C:309:ARG:HH11	1.78	0.49
1:B:335:ARG:NH1	1:B:335:ARG:CG	2.42	0.48
1:C:226:ARG:HD3	1:C:260:TRP:CG	2.48	0.48
1:B:40:SER:OG	1:B:101:GLU:HA	2.11	0.48
1:D:45:THR:O	1:D:45:THR:HG22	2.13	0.48
1:A:347:VAL:CG1	1:A:347:VAL:O	2.61	0.48
1:B:146:LEU:HD21	1:B:173:THR:OG1	2.13	0.48
1:D:103:SER:OG	1:D:303:PHE:CE1	2.61	0.48
1:A:120:ARG:HH11	1:A:120:ARG:HG2	1.77	0.48
1:C:419:GLN:HA	1:C:419:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:HB1	1:A:319:ALA:HB3	1.95	0.48
1:C:445:PHE:O	1:C:446:GLN:HG2	2.13	0.48
1:C:431:TYR:CD1	1:C:431:TYR:N	2.81	0.48
1:A:221:ILE:O	1:A:225:GLN:CG	2.60	0.48
1:B:399:HIS:NE2	1:B:403:ILE:HD11	2.26	0.48
1:A:424:TRP:NE1	1:A:464:TYR:HB2	2.29	0.48
1:D:406:ALA:HB1	1:D:442:LEU:HD21	1.95	0.48
1:D:471:ASP:OD2	1:D:471:ASP:N	2.43	0.48
1:D:290:PHE:CD2	1:D:304:PHE:HZ	2.32	0.48
1:B:286:THR:HG23	1:B:290:PHE:O	2.13	0.48
1:D:37:LEU:HD21	1:D:301:GLU:CG	2.44	0.48
1:C:90:ALA:HA	1:C:93:LEU:HD12	1.95	0.48
1:B:122:MSE:CE	1:B:180:PHE:CZ	2.97	0.48
1:C:108:VAL:CG2	1:C:134:GLN:HE21	2.27	0.48
1:C:127:ALA:HB2	1:C:149:GLU:CG	2.40	0.48
1:C:108:VAL:HG21	1:C:134:GLN:HE21	1.79	0.47
1:A:296:GLN:H	1:A:296:GLN:HG3	1.39	0.47
1:C:466:ARG:C	1:C:468:LEU:H	2.18	0.47
1:D:317:LEU:HB3	1:D:318:PRO:HD2	1.96	0.47
1:A:223:ALA:HA	1:A:226:ARG:HH12	1.72	0.47
1:B:199:GLY:O	1:B:202:VAL:HB	2.14	0.47
1:A:26:PHE:C	1:A:26:PHE:CD2	2.87	0.47
1:A:41:ILE:HG13	1:A:97:PHE:CD1	2.49	0.47
1:A:180:PHE:O	1:A:184:VAL:HG12	2.14	0.47
1:D:37:LEU:CD2	1:D:301:GLU:HG3	2.45	0.47
1:B:108:VAL:CG1	1:B:134:GLN:HG2	2.43	0.47
1:B:432:PRO:HG2	1:B:435:ALA:HA	1.97	0.47
1:D:273:PRO:HA	1:D:289:GLY:HA3	1.97	0.47
1:B:234:HIS:CE1	1:B:314:ILE:HD13	2.50	0.47
1:C:341:ARG:HD3	1:C:351:TRP:CZ2	2.47	0.47
1:D:260:TRP:O	1:D:263:GLU:HB2	2.15	0.47
1:A:42:ARG:NH2	1:A:134:GLN:HA	2.29	0.47
1:C:32:ALA:CB	1:C:296:GLN:HB3	2.45	0.47
1:C:32:ALA:HB2	1:C:296:GLN:HB3	1.97	0.47
1:A:45:THR:O	1:A:45:THR:CG2	2.60	0.47
1:B:184:VAL:O	1:B:185:PRO:O	2.32	0.47
1:B:296:GLN:HB2	1:B:296:GLN:HE21	1.53	0.47
1:A:198:SER:CB	1:A:218:ASN:HD21	2.26	0.47
1:B:136:SER:CB	1:B:167:ILE:HD12	2.45	0.47
1:D:445:PHE:C	1:D:446:GLN:HG2	2.35	0.47
1:D:234:HIS:HE1	1:D:265:TYR:OH	1.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ASN:OD1	1:C:412:ASN:N	2.48	0.47
1:D:210:LEU:HB2	1:D:213:TRP:HB2	1.96	0.46
1:C:37:LEU:HG	1:C:204:ARG:HB2	1.98	0.46
1:D:347:VAL:HG11	1:D:452:LEU:HD11	1.97	0.46
1:D:426:ARG:HH11	1:D:474:LEU:HD12	1.79	0.46
1:C:187:MSE:CE	1:C:187:MSE:HB2	2.45	0.46
1:D:459:ARG:O	1:D:460:LEU:HB2	2.15	0.46
1:C:336:GLU:HA	1:C:339:GLN:HG2	1.96	0.46
1:B:358:TRP:CD1	1:B:367:PHE:CD2	3.03	0.46
1:C:237:ARG:HG3	1:C:238:PRO:O	2.16	0.46
1:D:29:PHE:O	1:D:33:CYS:HB2	2.15	0.46
1:C:106:LEU:HB3	1:C:107:PRO:CD	2.44	0.46
1:C:111:LEU:HD23	1:C:112:PHE:CE2	2.51	0.46
1:C:366:LEU:O	1:C:384:GLY:HA3	2.16	0.46
1:C:35:ARG:HH21	1:C:299:ASP:CG	2.19	0.46
1:A:184:VAL:HG22	1:A:187:MSE:CB	2.46	0.46
1:D:424:TRP:NE1	1:D:464:TYR:HB2	2.30	0.46
1:A:246:THR:OG1	1:A:254:ASN:OD1	2.29	0.46
1:C:351:TRP:O	1:C:351:TRP:HE3	1.98	0.46
1:B:473:LYS:C	1:B:474:LEU:HG	2.36	0.46
1:D:122:MSE:HE3	1:D:146:LEU:HD22	1.95	0.46
1:D:338:GLY:HA2	1:D:341:ARG:HD2	1.97	0.46
1:D:167:ILE:HG21	1:D:170:VAL:HG23	1.98	0.46
1:D:357:LEU:HD12	1:D:357:LEU:N	2.31	0.46
1:C:362:LYS:H	1:C:362:LYS:HG2	1.43	0.46
1:B:55:GLN:HB3	1:B:55:GLN:HE21	1.57	0.46
1:D:101:GLU:HG2	1:D:101:GLU:H	1.33	0.46
1:D:42:ARG:HE	1:D:100:GLN:NE2	2.12	0.45
1:B:131:LYS:O	1:B:134:GLN:HB3	2.17	0.45
1:C:226:ARG:HG2	1:C:260:TRP:CE3	2.51	0.45
1:D:200:GLU:HG2	1:D:248:THR:OG1	2.16	0.45
1:D:464:TYR:HE2	1:D:469:VAL:HA	1.81	0.45
1:C:216:GLU:HA	1:C:216:GLU:OE2	2.16	0.45
1:A:146:LEU:HD11	1:A:173:THR:HG21	1.98	0.45
1:A:427:GLY:HA2	1:A:462:ASN:ND2	2.31	0.45
1:B:341:ARG:CB	1:B:351:TRP:HZ2	2.24	0.45
1:A:197:CYS:CB	1:A:248:THR:HG22	2.46	0.45
1:D:466:ARG:C	1:D:468:LEU:H	2.20	0.45
1:C:432:PRO:HG2	1:C:435:ALA:HA	1.98	0.45
1:A:35:ARG:HG3	1:A:204:ARG:HH21	1.81	0.45
1:B:321:LYS:HA	1:B:321:LYS:HD2	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LYS:O	1:A:390:THR:OG1	2.33	0.45
1:C:273:PRO:HA	1:C:289:GLY:HA3	1.99	0.45
1:C:199:GLY:O	1:C:202:VAL:HB	2.16	0.45
1:B:246:THR:OG1	1:B:254:ASN:ND2	2.37	0.45
1:D:432:PRO:HG2	1:D:435:ALA:HA	1.98	0.45
1:D:420:GLU:HG2	1:D:430:VAL:HG13	1.98	0.45
1:D:300:CYS:HB2	1:D:301:GLU:H	1.64	0.45
1:D:367:PHE:CE1	1:D:383:LEU:HB2	2.51	0.45
1:C:142:GLU:CA	1:C:142:GLU:OE2	2.65	0.45
1:D:8:PHE:HE1	1:D:34:GLN:HE22	1.65	0.45
1:B:184:VAL:O	1:B:184:VAL:HG12	2.17	0.44
1:D:347:VAL:CG1	1:D:452:LEU:HD11	2.47	0.44
1:A:233:PHE:CZ	1:A:269:VAL:HG22	2.52	0.44
1:B:226:ARG:HD2	1:B:260:TRP:CE2	2.52	0.44
1:A:329:PHE:CZ	1:A:360:ARG:NH1	2.86	0.44
1:C:65:THR:HB	1:C:75:TRP:HB2	1.99	0.44
1:D:146:LEU:HD23	1:D:146:LEU:C	2.37	0.44
1:C:341:ARG:HH11	1:C:351:TRP:HH2	1.65	0.44
1:C:367:PHE:CD1	1:C:383:LEU:HB2	2.52	0.44
1:C:296:GLN:HG3	1:C:296:GLN:H	1.39	0.44
1:B:56:LEU:HD11	1:B:446:GLN:HG2	2.00	0.44
1:A:20:MSE:HA	1:A:21:PRO:HD3	1.79	0.44
1:D:454:LYS:HB3	1:D:454:LYS:HE2	1.78	0.44
1:C:259:LEU:HD23	1:C:259:LEU:HA	1.71	0.44
1:A:423:GLU:HG3	1:A:428:ARG:HB2	2.00	0.44
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.65	0.44
1:B:456:ILE:HD12	1:B:459:ARG:HD2	1.99	0.44
1:C:202:VAL:CG1	1:C:202:VAL:O	2.65	0.44
1:B:386:LYS:HD2	1:B:398:GLN:HG3	2.00	0.44
1:A:259:LEU:HA	1:A:259:LEU:HD23	1.73	0.44
1:A:149:GLU:OE1	1:A:149:GLU:HA	2.18	0.44
1:C:415:GLU:OE1	1:C:445:PHE:HA	2.18	0.44
1:B:462:ASN:ND2	1:B:464:TYR:H	2.16	0.44
1:A:322:TYR:O	1:A:323:LYS:C	2.56	0.44
1:C:456:ILE:CG2	1:C:459:ARG:NH2	2.81	0.43
1:C:88:SER:HB3	1:C:470:ARG:HE	1.82	0.43
1:D:40:SER:OG	1:D:101:GLU:HA	2.17	0.43
1:C:446:GLN:HE21	1:C:446:GLN:HB3	1.64	0.43
1:B:39:ARG:H	1:B:39:ARG:HG3	1.55	0.43
1:B:86:LEU:CD2	1:B:97:PHE:CZ	3.01	0.43
1:C:186:GLU:HB2	1:C:237:ARG:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LEU:O	1:C:89:THR:HG22	2.18	0.43
1:A:347:VAL:HG12	1:A:347:VAL:O	2.17	0.43
1:B:386:LYS:HB3	1:B:398:GLN:HG3	1.99	0.43
1:C:374:LEU:HD12	1:C:374:LEU:N	2.33	0.43
1:B:112:PHE:CD2	1:B:112:PHE:N	2.86	0.43
1:B:356:ARG:HG2	1:B:356:ARG:NH1	2.34	0.43
1:D:135:ILE:O	1:D:139:MSE:HG3	2.19	0.43
1:C:236:LEU:O	1:C:310:LYS:CE	2.65	0.43
1:D:225:GLN:HE22	1:D:253:GLU:CG	2.27	0.43
1:A:169:ASN:HD22	1:A:170:VAL:HG23	1.84	0.43
1:B:357:LEU:H	1:B:357:LEU:HD12	1.84	0.43
1:C:120:ARG:NE	1:C:370:GLY:O	2.52	0.43
1:B:410:ASN:ND2	1:B:412:ASN:OD1	2.52	0.43
1:C:351:TRP:O	1:C:351:TRP:CE3	2.72	0.43
1:B:12:PHE:HE1	1:B:200:GLU:OE1	2.01	0.43
1:A:174:HIS:ND1	1:A:174:HIS:O	2.47	0.43
1:B:91:GLU:HG3	1:B:96:LEU:HD12	1.99	0.43
1:D:415:GLU:OE1	1:D:445:PHE:HA	2.19	0.43
1:B:294:PHE:H	1:B:297:ILE:CD1	2.31	0.43
1:A:328:PRO:HG2	1:A:329:PHE:CE1	2.53	0.43
1:B:13:LEU:C	1:B:15:GLN:H	2.22	0.43
1:D:357:LEU:HD12	1:D:357:LEU:H	1.83	0.43
1:C:69:TRP:CG	1:C:106:LEU:HD13	2.53	0.43
1:D:120:ARG:HH11	1:D:187:MSE:HG3	1.84	0.43
1:C:335:ARG:HB3	1:C:335:ARG:NH1	2.06	0.43
1:A:318:PRO:HB2	1:A:319:ALA:HA	2.00	0.43
1:C:9:PRO:HD3	1:C:210:LEU:HD13	2.01	0.43
1:D:427:GLY:HA2	1:D:462:ASN:OD1	2.19	0.43
1:D:272:LEU:CB	1:D:307:ARG:HE	2.32	0.42
1:B:294:PHE:H	1:B:297:ILE:HD12	1.83	0.42
1:C:424:TRP:HH2	1:C:453:ALA:HB2	1.84	0.42
1:B:296:GLN:H	1:B:296:GLN:HG3	1.34	0.42
1:C:366:LEU:HD11	1:C:387:LEU:HD22	2.02	0.42
1:C:466:ARG:O	1:C:469:VAL:HG22	2.20	0.42
1:B:112:PHE:HZ	1:B:135:ILE:HG23	1.84	0.42
1:C:158:LEU:HD23	1:C:162:ILE:HD12	2.00	0.42
1:D:371:ILE:HD12	1:D:374:LEU:CD1	2.49	0.42
1:D:214:SER:HB3	1:D:217:SER:HB3	2.00	0.42
1:D:409:ASP:N	1:D:409:ASP:OD1	2.53	0.42
1:D:272:LEU:HB2	1:D:307:ARG:HE	1.84	0.42
1:C:424:TRP:CH2	1:C:453:ALA:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:THR:HB	1:C:418:PRO:HD2	2.01	0.42
1:D:187:MSE:HB3	1:D:188:PHE:CD2	2.54	0.42
1:A:225:GLN:OE1	1:A:253:GLU:CG	2.55	0.42
1:A:37:LEU:HD11	1:A:301:GLU:HG3	2.00	0.42
1:D:225:GLN:NE2	1:D:253:GLU:HG2	2.30	0.42
1:A:473:LYS:N	1:A:473:LYS:HZ3	2.16	0.42
1:C:420:GLU:HG2	1:C:430:VAL:HG13	2.02	0.42
1:B:347:VAL:HG12	1:B:347:VAL:O	2.18	0.42
1:D:466:ARG:C	1:D:468:LEU:N	2.73	0.42
1:D:322:TYR:O	1:D:323:LYS:C	2.57	0.42
1:D:91:GLU:CD	1:D:91:GLU:H	2.22	0.42
1:C:233:PHE:CZ	1:C:310:LYS:HG3	2.54	0.42
1:B:210:LEU:HB2	1:B:213:TRP:HB2	2.02	0.42
1:B:86:LEU:CD2	1:B:97:PHE:CE1	3.02	0.42
1:C:20:MSE:HG2	1:C:26:PHE:HA	2.01	0.42
1:C:416:LEU:HD22	1:C:420:GLU:HB3	2.02	0.42
1:C:96:LEU:HD21	1:C:448:GLN:HG3	2.01	0.42
1:A:319:ALA:N	1:A:320:PRO:HD3	2.30	0.42
1:D:296:GLN:N	1:D:296:GLN:HE21	2.14	0.42
1:B:62:TRP:HE3	1:B:64:LEU:HD11	1.84	0.42
1:C:406:ALA:HB3	1:C:449:PRO:HB3	2.00	0.42
1:A:226:ARG:HG3	1:A:260:TRP:CE3	2.55	0.41
1:C:327:PHE:CD2	1:C:328:PRO:HD2	2.55	0.41
1:C:13:LEU:C	1:C:15:GLN:H	2.23	0.41
1:D:340:ILE:HD13	1:D:364:LEU:HD13	2.02	0.41
1:A:34:GLN:HB2	1:A:34:GLN:HE21	1.72	0.41
1:D:195:ALA:HA	1:D:196:PRO:HD3	1.95	0.41
1:C:206:ASP:HB3	1:C:209:ALA:HB2	2.02	0.41
1:A:101:GLU:HG2	1:A:101:GLU:H	1.63	0.41
1:B:131:LYS:NZ	1:B:194:ASP:OD1	2.29	0.41
1:B:385:ILE:HD11	1:B:405:LEU:HD21	2.03	0.41
1:D:309:ARG:HB3	1:D:309:ARG:HH11	1.85	0.41
1:A:169:ASN:HD22	1:A:169:ASN:C	2.22	0.41
1:C:466:ARG:C	1:C:468:LEU:N	2.74	0.41
1:A:454:LYS:NZ	1:A:454:LYS:HD2	2.36	0.41
1:C:184:VAL:HG22	1:C:187:MSE:HB2	2.01	0.41
1:A:416:LEU:HD13	1:A:421:ALA:HA	2.02	0.41
1:D:29:PHE:CD1	1:D:295:PRO:HD2	2.55	0.41
1:B:111:LEU:HD12	1:B:111:LEU:HA	1.85	0.41
1:A:222:ALA:HA	1:A:225:GLN:HG3	2.03	0.41
1:A:434:ALA:O	1:A:435:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:GLU:HB2	1:D:420:GLU:OE1	2.21	0.41
1:C:210:LEU:HB2	1:C:213:TRP:HB2	2.03	0.41
1:A:210:LEU:H	1:A:210:LEU:HG	1.63	0.41
1:B:422:GLU:HB3	1:B:426:ARG:NH2	2.36	0.41
1:C:422:GLU:HG3	1:C:474:LEU:HD12	2.02	0.41
1:B:65:THR:HA	1:B:66:PRO:HD3	1.91	0.41
1:C:321:LYS:HA	1:C:321:LYS:HD2	1.65	0.41
1:A:184:VAL:O	1:A:185:PRO:O	2.39	0.41
1:B:466:ARG:C	1:B:468:LEU:H	2.24	0.41
1:C:158:LEU:HD23	1:C:162:ILE:CD1	2.51	0.41
1:A:287:GLU:HG3	1:B:379:ARG:CD	2.51	0.41
1:D:12:PHE:HE1	1:D:200:GLU:OE1	2.04	0.41
1:A:146:LEU:HD11	1:A:173:THR:CG2	2.51	0.41
1:B:250:ASN:O	1:B:254:ASN:OD1	2.39	0.41
1:D:318:PRO:O	1:D:320:PRO:CG	2.68	0.41
1:C:162:ILE:HG23	1:C:167:ILE:HB	2.03	0.41
1:C:179:VAL:HG12	1:C:183:ALA:HB2	2.03	0.41
1:A:336:GLU:HA	1:A:339:GLN:HG2	2.03	0.41
1:D:122:MSE:HE1	1:D:180:PHE:CE2	2.55	0.40
1:B:409:ASP:N	1:B:409:ASP:OD1	2.55	0.40
1:C:184:VAL:N	1:C:185:PRO:CD	2.83	0.40
1:B:135:ILE:H	1:B:135:ILE:HG12	1.71	0.40
1:D:341:ARG:NE	1:D:351:TRP:CH2	2.86	0.40
1:A:167:ILE:CG2	1:A:170:VAL:HG23	2.52	0.40
1:A:162:ILE:HG23	1:A:167:ILE:HB	2.03	0.40
1:B:251:GLN:NE2	1:B:255:GLU:HB2	2.36	0.40
1:C:67:ILE:HA	1:C:68:PRO:HD3	1.97	0.40
1:D:146:LEU:HD21	1:D:173:THR:OG1	2.22	0.40
1:B:245:SER:HA	1:B:304:PHE:O	2.21	0.40
1:B:455:ARG:O	1:B:456:ILE:C	2.59	0.40
1:C:415:GLU:OE1	1:C:446:GLN:N	2.54	0.40
1:C:41:ILE:HG21	1:C:41:ILE:HD13	1.77	0.40
1:C:44:ASN:OD1	1:C:44:ASN:C	2.60	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	449/479 (94%)	408 (91%)	28 (6%)	13 (3%)	6	23
1	B	448/479 (94%)	401 (90%)	35 (8%)	12 (3%)	6	25
1	C	448/479 (94%)	401 (90%)	33 (7%)	14 (3%)	5	21
1	D	449/479 (94%)	403 (90%)	32 (7%)	14 (3%)	5	21
All	All	1794/1916 (94%)	1613 (90%)	128 (7%)	53 (3%)	5	22

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	PRO
1	A	211	LYS
1	A	409	ASP
1	B	185	PRO
1	B	211	LYS
1	B	319	ALA
1	C	185	PRO
1	C	211	LYS
1	C	319	ALA
1	C	456	ILE
1	D	185	PRO
1	D	211	LYS
1	D	319	ALA
1	A	177	GLY
1	A	456	ILE
1	A	467	GLU
1	B	177	GLY
1	B	335	ARG
1	B	456	ILE
1	C	177	GLY
1	C	299	ASP
1	C	409	ASP

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Mol	Chain	Res	Type
1	D	103	SER
1	D	177	GLY
1	D	409	ASP
1	D	456	ILE
1	A	323	LYS
1	A	434	ALA
1	B	299	ASP
1	B	409	ASP
1	B	434	ALA
1	C	467	GLU
1	D	323	LYS
1	D	467	GLU
1	A	300	CYS
1	C	300	CYS
1	C	323	LYS
1	C	434	ALA
1	C	460	LEU
1	D	434	ALA
1	B	467	GLU
1	C	273	PRO
1	C	320	PRO
1	D	273	PRO
1	A	320	PRO
1	A	460	LEU
1	A	408	PRO
1	D	370	GLY
1	D	375	ILE
1	A	436	PRO
1	B	320	PRO
1	B	408	PRO
1	D	408	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	373/385 (97%)	310 (83%)	63 (17%)	2 8
1	B	372/385 (97%)	314 (84%)	58 (16%)	3 10
1	C	372/385 (97%)	320 (86%)	52 (14%)	4 12
1	D	372/385 (97%)	322 (87%)	50 (13%)	5 13
All	All	1489/1540 (97%)	1266 (85%)	223 (15%)	3 11

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	15	GLN
1	A	17	ARG
1	A	30	LEU
1	A	33	CYS
1	A	35	ARG
1	A	41	ILE
1	A	54	LEU
1	A	75	TRP
1	A	101	GLU
1	A	103	SER
1	A	104	SER
1	A	106	LEU
1	A	130	SER
1	A	141	ASN
1	A	142	GLU
1	A	150	PHE
1	A	156	LYS
1	A	169	ASN
1	A	176	ASP
1	A	178	ARG
1	A	179	VAL
1	A	185	PRO
1	A	193	LEU
1	A	203	VAL
1	A	205	LYS
1	A	210	LEU
1	A	214	SER
1	A	218	ASN
1	A	220	GLU

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Mol	Chain	Res	Type
1	A	226	ARG
1	A	247	CYS
1	A	248	THR
1	A	252	GLU
1	A	263	GLU
1	A	303	PHE
1	A	322	TYR
1	A	324	VAL
1	A	333	LYS
1	A	335	ARG
1	A	336	GLU
1	A	341	ARG
1	A	342	GLN
1	A	351	TRP
1	A	353	GLU
1	A	362	LYS
1	A	372	GLU
1	A	379	ARG
1	A	390	THR
1	A	393	LYS
1	A	409	ASP
1	A	411	MSE
1	A	412	ASN
1	A	433	GLN
1	A	439	ASP
1	A	440	ASP
1	A	454	LYS
1	A	466	ARG
1	A	467	GLU
1	A	469	VAL
1	A	470	ARG
1	A	471	ASP
1	A	473	LYS
1	B	8	PHE
1	B	13	LEU
1	B	15	GLN
1	B	27	ASP
1	B	34	GLN
1	B	39	ARG
1	B	54	LEU
1	B	75	TRP
1	B	86	LEU

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Mol	Chain	Res	Type
1	B	101	GLU
1	B	103	SER
1	B	104	SER
1	B	112	PHE
1	B	131	LYS
1	B	141	ASN
1	B	153	SER
1	B	158	LEU
1	B	178	ARG
1	B	185	PRO
1	B	196	PRO
1	B	210	LEU
1	B	214	SER
1	B	216	GLU
1	B	219	GLN
1	B	228	LEU
1	B	237	ARG
1	B	252	GLU
1	B	262	LYS
1	B	273	PRO
1	B	283	LYS
1	B	296	GLN
1	B	303	PHE
1	B	321	LYS
1	B	330	SER
1	B	335	ARG
1	B	336	GLU
1	B	342	GLN
1	B	345	THR
1	B	350	ASN
1	B	351	TRP
1	B	353	GLU
1	B	357	LEU
1	B	362	LYS
1	B	379	ARG
1	B	381	SER
1	B	386	LYS
1	B	405	LEU
1	B	412	ASN
1	B	433	GLN
1	B	440	ASP
1	B	443	VAL

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Mol	Chain	Res	Type
1	B	450	ILE
1	B	459	ARG
1	B	462	ASN
1	B	467	GLU
1	B	469	VAL
1	B	471	ASP
1	B	473	LYS
1	C	8	PHE
1	C	15	GLN
1	C	17	ARG
1	C	18	GLU
1	C	54	LEU
1	C	75	TRP
1	C	88	SER
1	C	96	LEU
1	C	103	SER
1	C	106	LEU
1	C	142	GLU
1	C	149	GLU
1	C	153	SER
1	C	154	ARG
1	C	156	LYS
1	C	163	SER
1	C	186	GLU
1	C	210	LEU
1	C	212	ASN
1	C	250	ASN
1	C	251	GLN
1	C	270	GLU
1	C	273	PRO
1	C	296	GLN
1	C	303	PHE
1	C	321	LYS
1	C	322	TYR
1	C	330	SER
1	C	335	ARG
1	C	341	ARG
1	C	342	GLN
1	C	347	VAL
1	C	350	ASN
1	C	351	TRP
1	C	353	GLU

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Mol	Chain	Res	Type
1	C	361	ASP
1	C	362	LYS
1	C	379	ARG
1	C	383	LEU
1	C	392	ASN
1	C	393	LYS
1	C	411	MSE
1	C	426	ARG
1	C	431	TYR
1	C	446	GLN
1	C	447	HIS
1	C	454	LYS
1	C	462	ASN
1	C	466	ARG
1	C	468	LEU
1	C	470	ARG
1	C	473	LYS
1	D	33	CYS
1	D	34	GLN
1	D	37	LEU
1	D	41	ILE
1	D	75	TRP
1	D	89	THR
1	D	101	GLU
1	D	104	SER
1	D	106	LEU
1	D	119	GLN
1	D	132	THR
1	D	138	ARG
1	D	149	GLU
1	D	176	ASP
1	D	178	ARG
1	D	179	VAL
1	D	185	PRO
1	D	205	LYS
1	D	210	LEU
1	D	218	ASN
1	D	225	GLN
1	D	226	ARG
1	D	250	ASN
1	D	273	PRO
1	D	296	GLN

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Mol	Chain	Res	Type
1	D	300	CYS
1	D	303	PHE
1	D	308	LEU
1	D	323	LYS
1	D	324	VAL
1	D	342	GLN
1	D	352	ASP
1	D	353	GLU
1	D	361	ASP
1	D	362	LYS
1	D	382	ARG
1	D	390	THR
1	D	409	ASP
1	D	411	MSE
1	D	415	GLU
1	D	419	GLN
1	D	439	ASP
1	D	440	ASP
1	D	446	GLN
1	D	450	ILE
1	D	462	ASN
1	D	467	GLU
1	D	470	ARG
1	D	471	ASP
1	D	473	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	34	GLN
1	A	134	GLN
1	A	141	ASN
1	A	169	ASN
1	A	212	ASN
1	A	218	ASN
1	A	359	GLN
1	A	462	ASN
1	B	15	GLN
1	B	55	GLN
1	B	92	HIS
1	B	100	GLN

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Mol	Chain	Res	Type
1	B	119	GLN
1	B	141	ASN
1	B	251	GLN
1	B	254	ASN
1	B	296	GLN
1	B	312	GLN
1	B	399	HIS
1	B	410	ASN
1	B	419	GLN
1	B	448	GLN
1	B	462	ASN
1	C	15	GLN
1	C	134	GLN
1	C	218	ASN
1	C	250	ASN
1	C	254	ASN
1	C	312	GLN
1	C	342	GLN
1	C	392	ASN
1	C	412	ASN
1	C	446	GLN
1	C	462	ASN
1	D	34	GLN
1	D	44	ASN
1	D	55	GLN
1	D	100	GLN
1	D	218	ASN
1	D	225	GLN
1	D	234	HIS
1	D	250	ASN
1	D	254	ASN
1	D	296	GLN
1	D	342	GLN
1	D	410	ASN
1	D	433	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	448/479 (93%)	0.03	9 (2%)	68	64	52, 65, 70, 77	0
1	B	447/479 (93%)	-0.02	4 (0%)	85	84	51, 65, 70, 76	0
1	C	447/479 (93%)	-0.01	12 (2%)	58	52	51, 65, 70, 77	0
1	D	448/479 (93%)	0.10	16 (3%)	46	38	52, 65, 70, 76	0
All	All	1790/1916 (93%)	0.03	41 (2%)	64	59	51, 65, 70, 77	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	442	LEU	3.7
1	C	21	PRO	3.4
1	A	445	PHE	3.3
1	D	203	VAL	3.2
1	C	322	TYR	3.2
1	B	205	LYS	3.2
1	D	424	TRP	3.2
1	B	207	PRO	3.1
1	C	213	TRP	3.0
1	C	466	ARG	3.0
1	D	207	PRO	3.0
1	C	12	PHE	2.9
1	D	436	PRO	2.8
1	A	62	TRP	2.8
1	D	41	ILE	2.8
1	B	8	PHE	2.7
1	D	425	TYR	2.6
1	C	34	GLN	2.6
1	C	456	ILE	2.6
1	A	41	ILE	2.6
1	A	90	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	393	LYS	2.5
1	D	64	LEU	2.4
1	A	424	TRP	2.4
1	D	421	ALA	2.3
1	A	202	VAL	2.3
1	D	202	VAL	2.3
1	C	216	GLU	2.3
1	D	322	TYR	2.3
1	D	62	TRP	2.3
1	C	209	ALA	2.2
1	A	414	PHE	2.2
1	D	8	PHE	2.2
1	D	470	ARG	2.2
1	A	435	ALA	2.1
1	A	74	PHE	2.1
1	B	12	PHE	2.1
1	C	207	PRO	2.1
1	D	413	ALA	2.1
1	C	198	SER	2.0
1	D	434	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.