Full wwPDB X-ray Structure Validation Report (i)

Feb 4, 2024 – 03:51 PM EST

PDB ID	:	1R0V
Title	:	Structure Determination of the Dimeric Endonuclease in a Pseudo-face-centerd P21212 space group
Authors	:	Li, H.; Zhang, Y.
Deposited on	:	2003-09-23
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

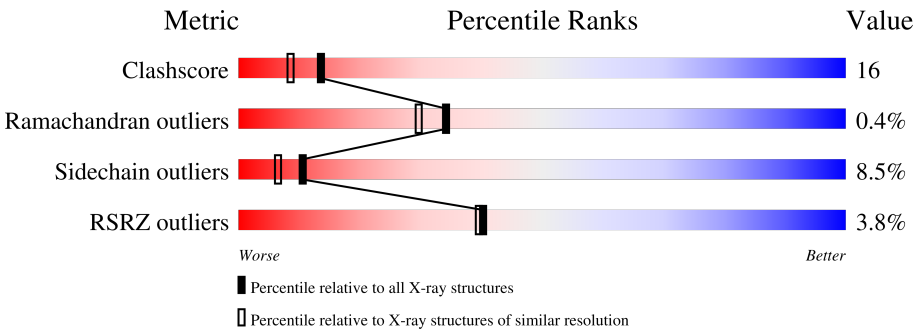
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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

Mol	Chain	Length	Quality of chain
1	A	305	2%, 42%, 30%, 6%, •, 20%
1	B	305	4%, 37%, 31%, 9%, •, 20%
1	C	305	3%, 43%, 28%, 7%, •, 20%
1	D	305	3%, 46%, 26%, 7%, •, 20%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9073 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 tRNA-intron endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	244	2050	1309	351	385	5	0	0	0
1	B	244	2050	1309	351	385	5	0	0	0
1	C	244	2050	1309	351	385	5	0	0	0
1	D	243	2042	1305	350	382	5	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	VAL	ILE	conflict	UNP O29362
B	152	VAL	ILE	conflict	UNP O29362
C	152	VAL	ILE	conflict	UNP O29362
D	152	VAL	ILE	conflict	UNP O29362

- Molecule 2 is water.

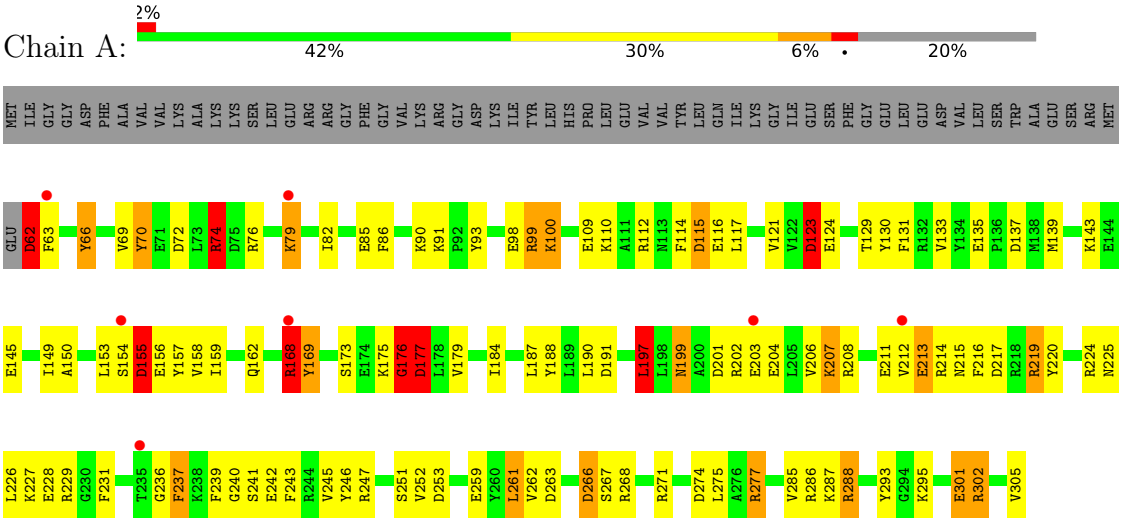
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	232	232	232	0	0
2	B	215	215	215	0	0
2	C	199	199	199	0	0
2	D	235	235	235	0	0

3 Residue-property plots (i)

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

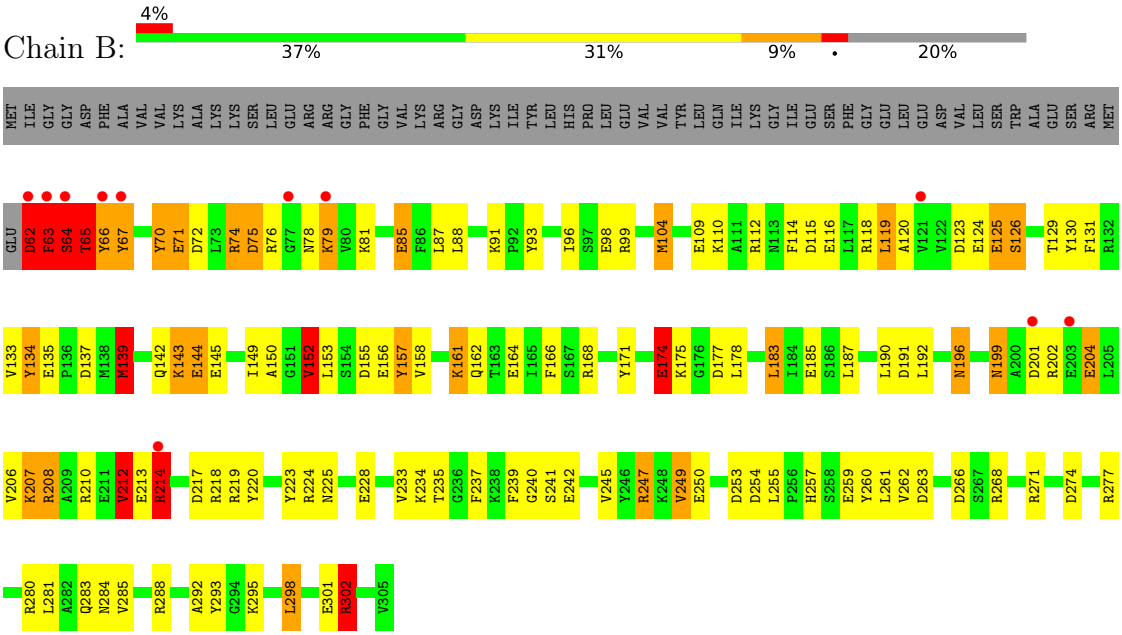
- Molecule 1: tRNA-intron endonuclease

Chain A:



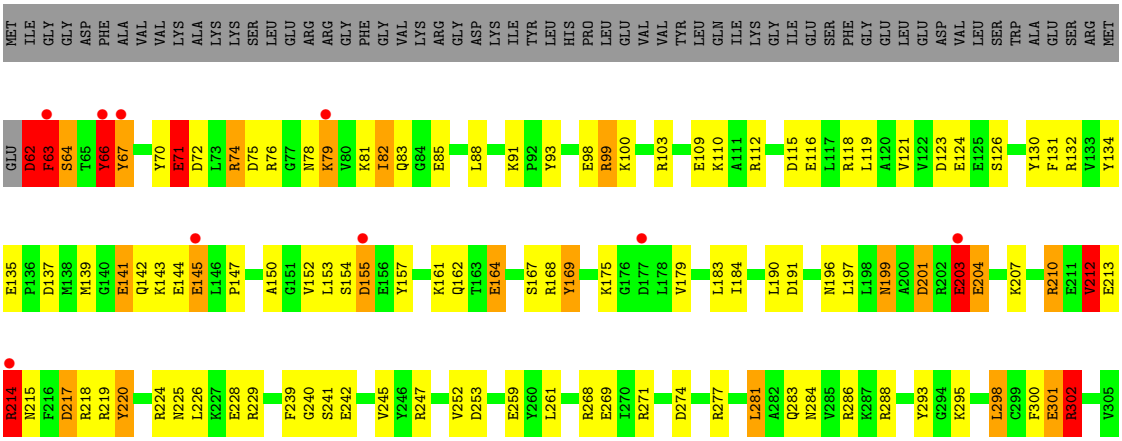
- Molecule 1: tRNA-intron endonuclease

Chain B:



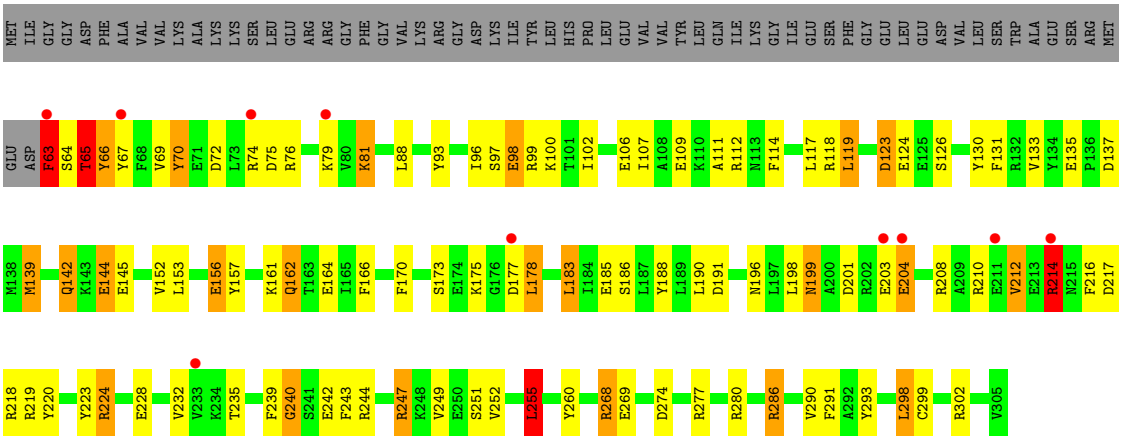
- Molecule 1: tRNA-intron endonuclease

Chain C:



- Molecule 1: tRNA-intron endonuclease

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.12Å 144.15Å 52.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.35 – 2.00 28.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.7 (95.35-2.00) 87.2 (28.13-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.62 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.174 , 0.242 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 60.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9073	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4528e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.94	52/2085 (2.5%)	1.77	63/2798 (2.3%)
1	B	2.30	106/2085 (5.1%)	2.20	116/2798 (4.1%)
1	C	2.27	86/2085 (4.1%)	2.22	97/2798 (3.5%)
1	D	2.00	56/2077 (2.7%)	1.85	58/2787 (2.1%)
All	All	2.13	300/8332 (3.6%)	2.02	334/11181 (3.0%)

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	B	0	4
1	C	0	1
1	D	0	1
All	All	0	6

All (300) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	124	GLU	CD-OE2	-13.79	1.10	1.25
1	B	144	GLU	CD-OE2	-12.54	1.11	1.25
1	A	157	TYR	CE1-CZ	-12.37	1.22	1.38
1	B	63	PHE	CB-CG	-12.15	1.30	1.51
1	C	70	TYR	CE2-CZ	-12.14	1.22	1.38
1	D	144	GLU	CD-OE2	12.09	1.39	1.25
1	B	70	TYR	CE2-CZ	-11.87	1.23	1.38
1	C	144	GLU	CD-OE2	-11.39	1.13	1.25
1	D	157	TYR	CE2-CZ	-11.29	1.23	1.38
1	D	67	TYR	CB-CG	-11.26	1.34	1.51
1	C	93	TYR	CD1-CE1	11.19	1.56	1.39
1	C	135	GLU	CD-OE2	-11.00	1.13	1.25
1	C	268	ARG	CZ-NH2	-10.78	1.19	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	TYR	CE1-CZ	-10.76	1.24	1.38
1	C	212	VAL	CB-CG2	-10.57	1.30	1.52
1	C	131	PHE	CE1-CZ	-10.51	1.17	1.37
1	C	67	TYR	CB-CG	-10.43	1.36	1.51
1	B	71	GLU	CD-OE1	-10.32	1.14	1.25
1	B	239	PHE	CG-CD2	-10.32	1.23	1.38
1	C	157	TYR	CE1-CZ	-10.18	1.25	1.38
1	B	76	ARG	CZ-NH1	-10.18	1.19	1.33
1	B	157	TYR	CE2-CZ	-10.06	1.25	1.38
1	C	130	TYR	CG-CD1	-10.05	1.26	1.39
1	C	212	VAL	CB-CG1	-9.76	1.32	1.52
1	B	66	TYR	CG-CD1	-9.69	1.26	1.39
1	A	66	TYR	CE2-CZ	-9.62	1.26	1.38
1	A	242	GLU	CD-OE1	-9.53	1.15	1.25
1	C	98	GLU	CD-OE1	-9.49	1.15	1.25
1	A	135	GLU	CD-OE1	-9.28	1.15	1.25
1	C	70	TYR	CG-CD2	-9.22	1.27	1.39
1	B	124	GLU	CD-OE2	-9.22	1.15	1.25
1	D	124	GLU	CD-OE1	-9.20	1.15	1.25
1	B	70	TYR	CG-CD2	-9.18	1.27	1.39
1	C	152	VAL	CB-CG2	-9.14	1.33	1.52
1	C	70	TYR	CG-CD1	-9.14	1.27	1.39
1	C	157	TYR	CE2-CZ	-9.10	1.26	1.38
1	A	66	TYR	CB-CG	-9.04	1.38	1.51
1	B	228	GLU	CD-OE1	-8.96	1.15	1.25
1	B	239	PHE	CE1-CZ	-8.91	1.20	1.37
1	B	157	TYR	CG-CD2	-8.82	1.27	1.39
1	B	66	TYR	CD1-CE1	-8.79	1.26	1.39
1	B	64	SER	CA-CB	-8.76	1.39	1.52
1	C	239	PHE	CE1-CZ	-8.73	1.20	1.37
1	B	135	GLU	CD-OE1	-8.69	1.16	1.25
1	C	135	GLU	CD-OE1	-8.66	1.16	1.25
1	B	124	GLU	CD-OE1	-8.65	1.16	1.25
1	C	259	GLU	CD-OE2	-8.60	1.16	1.25
1	C	242	GLU	CD-OE2	-8.59	1.16	1.25
1	B	66	TYR	CB-CG	-8.56	1.38	1.51
1	B	135	GLU	CD-OE2	-8.49	1.16	1.25
1	D	114	PHE	CG-CD2	-8.49	1.26	1.38
1	C	169	TYR	CD1-CE1	8.45	1.52	1.39
1	D	293	TYR	CD2-CE2	8.32	1.51	1.39
1	B	98	GLU	CD-OE2	-8.25	1.16	1.25
1	B	161	LYS	CD-CE	8.22	1.71	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	93	TYR	CG-CD1	-8.16	1.28	1.39
1	D	218	ARG	CG-CD	8.16	1.72	1.51
1	A	121	VAL	CB-CG1	8.12	1.70	1.52
1	C	284	ASN	CG-OD1	-8.10	1.06	1.24
1	C	66	TYR	CB-CG	-8.07	1.39	1.51
1	B	212	VAL	CB-CG2	-8.06	1.35	1.52
1	B	67	TYR	CE2-CZ	-8.05	1.28	1.38
1	B	223	TYR	CD1-CE1	7.96	1.51	1.39
1	B	213	GLU	CD-OE1	-7.96	1.16	1.25
1	C	210	ARG	CZ-NH1	-7.92	1.22	1.33
1	B	64	SER	CA-C	-7.89	1.32	1.52
1	D	70	TYR	CE1-CZ	-7.86	1.28	1.38
1	B	109	GLU	CG-CD	7.85	1.63	1.51
1	B	70	TYR	CE1-CZ	-7.84	1.28	1.38
1	B	234	LYS	CD-CE	7.83	1.70	1.51
1	C	124	GLU	CD-OE1	-7.82	1.17	1.25
1	C	99	ARG	CZ-NH1	-7.77	1.23	1.33
1	C	300	PHE	CE1-CZ	7.77	1.52	1.37
1	B	66	TYR	CE2-CZ	-7.70	1.28	1.38
1	D	260	TYR	CD2-CE2	7.70	1.50	1.39
1	C	239	PHE	CD1-CE1	7.64	1.54	1.39
1	B	62	ASP	CA-CB	7.58	1.70	1.53
1	C	130	TYR	CE2-CZ	-7.54	1.28	1.38
1	B	285	VAL	CB-CG2	7.51	1.68	1.52
1	C	220	TYR	CE1-CZ	7.51	1.48	1.38
1	B	301	GLU	CB-CG	-7.49	1.38	1.52
1	B	219	ARG	CZ-NH1	-7.43	1.23	1.33
1	D	170	PHE	CD1-CE1	-7.42	1.24	1.39
1	C	64	SER	CA-CB	-7.41	1.41	1.52
1	B	93	TYR	CE2-CZ	-7.41	1.28	1.38
1	D	66	TYR	CB-CG	-7.40	1.40	1.51
1	A	66	TYR	CG-CD1	-7.37	1.29	1.39
1	C	157	TYR	CG-CD2	-7.34	1.29	1.39
1	B	70	TYR	CG-CD1	-7.31	1.29	1.39
1	A	139	MET	CG-SD	-7.28	1.62	1.81
1	B	75	ASP	CB-CG	-7.22	1.36	1.51
1	D	93	TYR	CD2-CE2	7.15	1.50	1.39
1	A	69	VAL	CB-CG1	7.08	1.67	1.52
1	A	252	VAL	CA-CB	7.06	1.69	1.54
1	C	131	PHE	CD1-CE1	7.03	1.53	1.39
1	C	82	ILE	CB-CG2	-6.99	1.31	1.52
1	A	116	GLU	CD-OE1	-6.97	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	71	GLU	CB-CG	-6.97	1.39	1.52
1	C	228	GLU	CD-OE1	-6.93	1.18	1.25
1	D	70	TYR	CG-CD2	-6.92	1.30	1.39
1	A	130	TYR	CE2-CZ	-6.91	1.29	1.38
1	D	81	LYS	CD-CE	6.90	1.68	1.51
1	A	267	SER	CB-OG	-6.90	1.33	1.42
1	C	71	GLU	CD-OE1	-6.88	1.18	1.25
1	B	292	ALA	CA-CB	6.87	1.66	1.52
1	B	93	TYR	CG-CD1	-6.86	1.30	1.39
1	B	157	TYR	CG-CD1	-6.86	1.30	1.39
1	A	86	PHE	CE2-CZ	-6.84	1.24	1.37
1	A	131	PHE	CD1-CE1	6.83	1.52	1.39
1	D	64	SER	CA-CB	-6.78	1.42	1.52
1	A	124	GLU	CD-OE2	-6.77	1.18	1.25
1	B	130	TYR	CG-CD2	-6.77	1.30	1.39
1	B	281	LEU	CG-CD1	-6.74	1.26	1.51
1	D	219	ARG	CG-CD	6.73	1.68	1.51
1	A	86	PHE	CD1-CE1	6.72	1.52	1.39
1	D	76	ARG	CZ-NH2	-6.69	1.24	1.33
1	D	64	SER	N-CA	-6.68	1.32	1.46
1	C	145	GLU	CD-OE2	-6.68	1.18	1.25
1	B	64	SER	CB-OG	6.67	1.50	1.42
1	C	203	GLU	CD-OE1	6.65	1.32	1.25
1	B	268	ARG	CZ-NH2	-6.63	1.24	1.33
1	B	63	PHE	N-CA	6.62	1.59	1.46
1	D	109	GLU	CG-CD	6.59	1.61	1.51
1	C	109	GLU	CG-CD	6.54	1.61	1.51
1	C	226	LEU	N-CA	6.52	1.59	1.46
1	B	293	TYR	CD1-CE1	6.50	1.49	1.39
1	D	114	PHE	CE1-CZ	-6.49	1.25	1.37
1	A	124	GLU	CD-OE1	-6.44	1.18	1.25
1	C	141	GLU	CD-OE2	6.43	1.32	1.25
1	D	177	ASP	C-O	6.43	1.35	1.23
1	A	231	PHE	CE2-CZ	6.43	1.49	1.37
1	B	131	PHE	CD1-CE1	6.40	1.52	1.39
1	B	62	ASP	N-CA	6.39	1.59	1.46
1	B	134	TYR	CE1-CZ	-6.39	1.30	1.38
1	A	98	GLU	CD-OE1	-6.39	1.18	1.25
1	B	241	SER	CA-CB	6.37	1.62	1.52
1	C	93	TYR	CE1-CZ	-6.36	1.30	1.38
1	D	290	VAL	CB-CG2	6.36	1.66	1.52
1	B	237	PHE	CE1-CZ	6.35	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	VAL	CB-CG1	-6.33	1.39	1.52
1	B	225	ASN	CG-OD1	-6.33	1.10	1.24
1	D	268	ARG	CZ-NH2	-6.28	1.24	1.33
1	D	178	LEU	CG-CD1	-6.27	1.28	1.51
1	B	114	PHE	CG-CD2	-6.25	1.29	1.38
1	C	109	GLU	CD-OE2	6.25	1.32	1.25
1	D	218	ARG	CB-CG	-6.24	1.35	1.52
1	C	252	VAL	CA-CB	6.24	1.67	1.54
1	A	219	ARG	CG-CD	6.21	1.67	1.51
1	A	237	PHE	CD1-CE1	6.17	1.51	1.39
1	D	65	THR	CB-CG2	-6.17	1.31	1.52
1	B	283	GLN	CD-OE1	-6.16	1.10	1.24
1	D	214	ARG	C-O	-6.15	1.11	1.23
1	B	67	TYR	CB-CG	-6.14	1.42	1.51
1	A	239	PHE	CD1-CE1	6.12	1.51	1.39
1	D	186	SER	CB-OG	6.11	1.50	1.42
1	C	131	PHE	CG-CD2	-6.10	1.29	1.38
1	C	219	ARG	CZ-NH2	-6.10	1.25	1.33
1	B	130	TYR	CG-CD1	-6.07	1.31	1.39
1	C	76	ARG	CZ-NH2	-6.06	1.25	1.33
1	A	243	PHE	CE2-CZ	-6.05	1.25	1.37
1	B	218	ARG	CG-CD	6.04	1.67	1.51
1	C	288	ARG	CB-CG	6.02	1.68	1.52
1	C	242	GLU	CD-OE1	-6.01	1.19	1.25
1	C	99	ARG	CZ-NH2	-6.01	1.25	1.33
1	B	259	GLU	CD-OE1	-6.00	1.19	1.25
1	D	166	PHE	CD2-CE2	5.98	1.51	1.39
1	A	91	LYS	CE-NZ	-5.96	1.34	1.49
1	A	86	PHE	CG-CD2	-5.95	1.29	1.38
1	B	196	ASN	CB-CG	-5.94	1.37	1.51
1	B	242	GLU	CD-OE1	-5.93	1.19	1.25
1	B	250	GLU	CD-OE1	5.91	1.32	1.25
1	B	220	TYR	CE2-CZ	5.90	1.46	1.38
1	B	271	ARG	CZ-NH2	-5.89	1.25	1.33
1	D	291	PHE	CD2-CE2	5.88	1.51	1.39
1	A	188	TYR	CD1-CE1	5.88	1.48	1.39
1	B	158	VAL	CB-CG2	5.88	1.65	1.52
1	C	184	ILE	CB-CG2	5.86	1.71	1.52
1	C	220	TYR	CD2-CE2	5.86	1.48	1.39
1	B	249	VAL	CB-CG1	5.84	1.65	1.52
1	C	247	ARG	CZ-NH2	-5.84	1.25	1.33
1	D	223	TYR	CD2-CE2	5.83	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	100	LYS	C-O	5.81	1.34	1.23
1	D	243	PHE	CD2-CE2	-5.81	1.27	1.39
1	B	271	ARG	CZ-NH1	-5.80	1.25	1.33
1	A	285	VAL	CB-CG1	5.78	1.65	1.52
1	B	65	THR	CB-CG2	-5.76	1.33	1.52
1	D	70	TYR	CG-CD1	-5.76	1.31	1.39
1	C	144	GLU	CD-OE1	-5.76	1.19	1.25
1	B	119	LEU	CG-CD2	-5.71	1.30	1.51
1	D	109	GLU	CD-OE2	5.71	1.31	1.25
1	D	131	PHE	CD1-CE1	5.69	1.50	1.39
1	B	76	ARG	CZ-NH2	-5.68	1.25	1.33
1	A	179	VAL	CB-CG2	5.67	1.64	1.52
1	B	120	ALA	CA-CB	5.66	1.64	1.52
1	C	283	GLN	CD-OE1	-5.66	1.11	1.24
1	A	66	TYR	CD2-CE2	-5.63	1.30	1.39
1	B	171	TYR	CE2-CZ	5.63	1.45	1.38
1	C	66	TYR	CG-CD1	-5.61	1.31	1.39
1	B	185	GLU	CD-OE1	5.60	1.31	1.25
1	A	169	TYR	CD2-CE2	5.60	1.47	1.39
1	A	169	TYR	CZ-OH	5.60	1.47	1.37
1	C	67	TYR	CA-CB	-5.60	1.41	1.53
1	C	142	GLN	CD-OE1	-5.59	1.11	1.24
1	A	93	TYR	CG-CD1	-5.59	1.31	1.39
1	C	252	VAL	CB-CG1	5.59	1.64	1.52
1	A	245	VAL	CB-CG2	5.58	1.64	1.52
1	D	106	GLU	CD-OE1	-5.58	1.19	1.25
1	D	239	PHE	CD2-CE2	5.57	1.50	1.39
1	C	63	PHE	CE1-CZ	5.57	1.48	1.37
1	A	216	PHE	CE2-CZ	5.57	1.48	1.37
1	B	259	GLU	CD-OE2	-5.55	1.19	1.25
1	C	63	PHE	C-N	-5.55	1.21	1.34
1	A	241	SER	CA-CB	5.55	1.61	1.52
1	D	239	PHE	CE1-CZ	-5.54	1.26	1.37
1	B	210	ARG	CZ-NH1	-5.53	1.25	1.33
1	C	269	GLU	CD-OE1	5.53	1.31	1.25
1	A	251	SER	CB-OG	-5.50	1.35	1.42
1	D	173	SER	CA-CB	5.50	1.61	1.52
1	D	232	VAL	CB-CG1	5.49	1.64	1.52
1	A	70	TYR	CB-CG	-5.49	1.43	1.51
1	C	241	SER	CB-OG	5.49	1.49	1.42
1	C	228	GLU	CD-OE2	-5.48	1.19	1.25
1	C	302	ARG	CZ-NH1	5.45	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	293	TYR	CG-CD2	5.45	1.46	1.39
1	B	85	GLU	CD-OE1	-5.45	1.19	1.25
1	B	130	TYR	CE2-CZ	-5.45	1.31	1.38
1	C	157	TYR	CG-CD1	-5.44	1.32	1.39
1	B	78	ASN	CG-OD1	-5.44	1.11	1.24
1	B	285	VAL	CA-CB	5.42	1.66	1.54
1	A	227	LYS	CE-NZ	5.41	1.62	1.49
1	A	149	ILE	CB-CG2	5.41	1.69	1.52
1	A	227	LYS	CD-CE	5.41	1.64	1.51
1	C	98	GLU	CD-OE2	-5.41	1.19	1.25
1	A	158	VAL	CB-CG2	5.40	1.64	1.52
1	B	67	TYR	CG-CD2	-5.40	1.32	1.39
1	D	69	VAL	CB-CG2	5.40	1.64	1.52
1	D	185	GLU	CD-OE2	5.39	1.31	1.25
1	A	305	VAL	CB-CG2	5.39	1.64	1.52
1	D	126	SER	CA-CB	5.38	1.61	1.52
1	B	155	ASP	CB-CG	-5.38	1.40	1.51
1	B	174	GLU	CB-CG	-5.37	1.42	1.52
1	B	271	ARG	CG-CD	5.37	1.65	1.51
1	A	114	PHE	CG-CD1	-5.35	1.30	1.38
1	B	161	LYS	CE-NZ	5.35	1.62	1.49
1	A	208	ARG	NE-CZ	5.33	1.40	1.33
1	B	207	LYS	CD-CE	5.30	1.64	1.51
1	B	233	VAL	CB-CG1	5.29	1.64	1.52
1	C	242	GLU	CG-CD	-5.29	1.44	1.51
1	D	157	TYR	CG-CD1	-5.29	1.32	1.39
1	B	62	ASP	CA-C	5.29	1.66	1.52
1	C	91	LYS	CB-CG	5.27	1.66	1.52
1	B	125	GLU	CD-OE2	5.25	1.31	1.25
1	C	207	LYS	CD-CE	5.24	1.64	1.51
1	B	262	VAL	CB-CG2	5.23	1.63	1.52
1	B	145	GLU	CD-OE2	-5.23	1.20	1.25
1	C	91	LYS	CE-NZ	-5.22	1.35	1.49
1	C	167	SER	CA-CB	5.22	1.60	1.52
1	D	216	PHE	CE2-CZ	5.22	1.47	1.37
1	C	63	PHE	CG-CD2	5.21	1.46	1.38
1	A	109	GLU	CG-CD	5.20	1.59	1.51
1	D	164	GLU	CD-OE1	5.20	1.31	1.25
1	B	116	GLU	CD-OE1	-5.20	1.20	1.25
1	D	70	TYR	CD1-CE1	5.19	1.47	1.39
1	B	104	MET	SD-CE	5.19	2.06	1.77
1	B	66	TYR	CE1-CZ	-5.18	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	VAL	CB-CG1	-5.18	1.42	1.52
1	D	212	VAL	CB-CG1	-5.17	1.42	1.52
1	B	239	PHE	CD2-CE2	5.16	1.49	1.39
1	D	224	ARG	CG-CD	-5.16	1.39	1.51
1	B	62	ASP	C-N	5.16	1.46	1.34
1	B	234	LYS	CE-NZ	5.16	1.61	1.49
1	B	144	GLU	CD-OE1	-5.15	1.20	1.25
1	D	240	GLY	C-O	5.15	1.31	1.23
1	B	99	ARG	CZ-NH1	-5.14	1.26	1.33
1	C	64	SER	CA-C	-5.14	1.39	1.52
1	A	246	TYR	CD1-CE1	5.13	1.47	1.39
1	D	242	GLU	CD-OE2	-5.13	1.20	1.25
1	B	126	SER	CA-CB	5.13	1.60	1.52
1	B	98	GLU	CD-OE1	-5.12	1.20	1.25
1	D	162	GLN	CD-OE1	-5.12	1.12	1.24
1	C	142	GLN	C-O	-5.12	1.13	1.23
1	D	255	LEU	CG-CD2	-5.11	1.32	1.51
1	C	210	ARG	CZ-NH2	-5.11	1.26	1.33
1	A	130	TYR	CD2-CE2	5.10	1.47	1.39
1	B	131	PHE	CG-CD2	-5.10	1.31	1.38
1	B	284	ASN	CG-ND2	-5.10	1.20	1.32
1	D	130	TYR	CE2-CZ	-5.08	1.31	1.38
1	B	133	VAL	CB-CG1	5.07	1.63	1.52
1	A	287	LYS	CD-CE	5.06	1.63	1.51
1	B	285	VAL	CB-CG1	5.06	1.63	1.52
1	D	299	CYS	C-O	5.05	1.32	1.23
1	C	245	VAL	CB-CG1	5.05	1.63	1.52
1	A	69	VAL	CB-CG2	5.04	1.63	1.52
1	B	242	GLU	CD-OE2	-5.04	1.20	1.25
1	C	131	PHE	CD2-CE2	5.04	1.49	1.39
1	C	215	ASN	CG-OD1	5.03	1.35	1.24
1	A	262	VAL	CB-CG2	5.02	1.63	1.52
1	A	70	TYR	CG-CD2	-5.01	1.32	1.39
1	C	78	ASN	CG-ND2	-5.00	1.20	1.32
1	C	179	VAL	CB-CG2	5.00	1.63	1.52

All (334) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	268	ARG	NE-CZ-NH1	32.39	136.50	120.30
1	C	268	ARG	NE-CZ-NH2	-24.40	108.10	120.30
1	D	268	ARG	NE-CZ-NH1	21.44	131.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	PHE	N-CA-C	-19.17	59.24	111.00
1	B	63	PHE	C-N-CA	-19.16	73.79	121.70
1	C	137	ASP	CB-CG-OD2	16.48	133.13	118.30
1	B	268	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	C	274	ASP	CB-CG-OD2	15.03	131.83	118.30
1	D	214	ARG	NE-CZ-NH2	-15.01	112.80	120.30
1	C	210	ARG	NE-CZ-NH2	14.57	127.59	120.30
1	B	64	SER	N-CA-CB	-14.37	88.94	110.50
1	C	214	ARG	NE-CZ-NH1	-14.23	113.19	120.30
1	B	214	ARG	NE-CZ-NH2	-13.92	113.34	120.30
1	C	103	ARG	NE-CZ-NH2	13.82	127.21	120.30
1	C	214	ARG	NE-CZ-NH2	13.75	127.18	120.30
1	B	137	ASP	CB-CG-OD1	13.24	130.21	118.30
1	D	268	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	D	218	ARG	NE-CZ-NH2	-12.81	113.90	120.30
1	B	214	ARG	NE-CZ-NH1	12.74	126.67	120.30
1	B	62	ASP	CB-CG-OD2	12.74	129.76	118.30
1	D	64	SER	N-CA-CB	-12.65	91.53	110.50
1	B	135	GLU	OE1-CD-OE2	-12.64	108.14	123.30
1	C	219	ARG	NE-CZ-NH1	12.11	126.35	120.30
1	C	72	ASP	CB-CG-OD2	11.95	129.05	118.30
1	D	214	ARG	NE-CZ-NH1	11.93	126.26	120.30
1	C	99	ARG	NE-CZ-NH2	11.91	126.26	120.30
1	C	124	GLU	OE1-CD-OE2	-11.91	109.00	123.30
1	C	191	ASP	CB-CG-OD1	11.69	128.82	118.30
1	B	271	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	B	253	ASP	CB-CG-OD2	11.55	128.69	118.30
1	A	268	ARG	NE-CZ-NH1	-11.51	114.54	120.30
1	B	201	ASP	CB-CG-OD2	11.48	128.63	118.30
1	A	266	ASP	CB-CG-OD2	11.47	128.62	118.30
1	A	208	ARG	NE-CZ-NH2	11.44	126.02	120.30
1	A	214	ARG	NE-CZ-NH2	11.25	125.92	120.30
1	B	74	ARG	NE-CZ-NH2	11.23	125.91	120.30
1	A	214	ARG	NE-CZ-NH1	-11.22	114.69	120.30
1	B	219	ARG	NE-CZ-NH2	11.19	125.89	120.30
1	C	63	PHE	C-N-CA	-11.10	93.94	121.70
1	D	191	ASP	CB-CG-OD2	11.05	128.25	118.30
1	B	98	GLU	OE1-CD-OE2	-11.00	110.10	123.30
1	B	76	ARG	NE-CZ-NH2	10.97	125.79	120.30
1	D	201	ASP	CB-CG-OD2	10.87	128.09	118.30
1	A	253	ASP	CB-CG-OD2	10.71	127.94	118.30
1	C	259	GLU	OE1-CD-OE2	-10.20	111.06	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	123	ASP	CB-CG-OD2	10.16	127.45	118.30
1	C	74	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	B	259	GLU	OE1-CD-OE2	-10.06	111.23	123.30
1	C	74	ARG	NE-CZ-NH1	9.98	125.29	120.30
1	D	217	ASP	CB-CG-OD2	9.96	127.27	118.30
1	B	137	ASP	OD1-CG-OD2	-9.95	104.39	123.30
1	B	210	ARG	NE-CZ-NH2	9.93	125.27	120.30
1	D	183	LEU	CB-CG-CD1	9.91	127.85	111.00
1	B	116	GLU	OE1-CD-OE2	-9.88	111.44	123.30
1	C	123	ASP	CB-CG-OD2	9.83	127.15	118.30
1	D	224	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	C	212	VAL	CG1-CB-CG2	-9.71	95.37	110.90
1	C	228	GLU	OE1-CD-OE2	-9.71	111.65	123.30
1	C	82	ILE	CG1-CB-CG2	-9.69	90.09	111.40
1	A	137	ASP	CB-CG-OD2	9.64	126.97	118.30
1	B	64	SER	CB-CA-C	9.63	128.39	110.10
1	A	202	ARG	NE-CZ-NH2	9.47	125.04	120.30
1	B	213	GLU	OE1-CD-OE2	-9.43	111.98	123.30
1	B	212	VAL	CG1-CB-CG2	-9.34	95.95	110.90
1	B	124	GLU	OE1-CD-OE2	-9.28	112.17	123.30
1	C	274	ASP	OD1-CG-OD2	-9.24	105.75	123.30
1	C	253	ASP	CB-CG-OD2	9.16	126.55	118.30
1	C	271	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	116	GLU	OE1-CD-OE2	-9.11	112.37	123.30
1	B	253	ASP	OD1-CG-OD2	-9.09	106.02	123.30
1	B	64	SER	CA-CB-OG	-9.08	86.69	111.20
1	D	112	ARG	NE-CZ-NH1	-8.99	115.80	120.30
1	A	191	ASP	CB-CG-OD2	8.89	126.30	118.30
1	B	112	ARG	NE-CZ-NH2	-8.89	115.86	120.30
1	D	135	GLU	OE1-CD-OE2	-8.85	112.68	123.30
1	C	135	GLU	OE1-CD-OE2	-8.85	112.68	123.30
1	B	118	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	B	63	PHE	N-CA-CB	-8.82	94.71	110.60
1	C	144	GLU	OE1-CD-OE2	-8.73	112.82	123.30
1	A	74	ARG	NE-CZ-NH1	-8.71	115.94	120.30
1	B	266	ASP	CB-CG-OD2	8.71	126.14	118.30
1	C	201	ASP	CB-CG-OD2	8.70	126.13	118.30
1	A	271	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	A	74	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	C	74	ARG	CG-CD-NE	-8.66	93.61	111.80
1	B	219	ARG	NH1-CZ-NH2	-8.60	109.95	119.40
1	D	247	ARG	NE-CZ-NH1	8.59	124.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	72	ASP	CB-CG-OD2	8.57	126.01	118.30
1	C	137	ASP	OD1-CG-OD2	-8.55	107.05	123.30
1	A	99	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	B	152	VAL	CA-CB-CG1	8.51	123.66	110.90
1	B	191	ASP	CB-CG-OD1	8.44	125.89	118.30
1	B	271	ARG	NH1-CZ-NH2	-8.44	110.12	119.40
1	A	177	ASP	CB-CG-OD1	8.38	125.84	118.30
1	B	63	PHE	CB-CG-CD1	-8.37	114.94	120.80
1	C	76	ARG	NE-CZ-NH2	8.35	124.47	120.30
1	B	177	ASP	CB-CG-OD2	8.34	125.80	118.30
1	A	72	ASP	CB-CG-OD2	8.33	125.80	118.30
1	C	191	ASP	OD1-CG-OD2	-8.27	107.59	123.30
1	A	261	LEU	CB-CG-CD2	8.05	124.68	111.00
1	A	124	GLU	OE1-CD-OE2	-8.03	113.67	123.30
1	A	201	ASP	CB-CG-OD2	7.95	125.45	118.30
1	D	255	LEU	CB-CG-CD1	7.87	124.38	111.00
1	A	261	LEU	CB-CG-CD1	7.86	124.36	111.00
1	B	137	ASP	CB-CG-OD2	7.85	125.37	118.30
1	B	261	LEU	CD1-CG-CD2	-7.80	87.11	110.50
1	B	76	ARG	NH1-CZ-NH2	-7.79	110.83	119.40
1	D	137	ASP	CB-CG-OD1	7.76	125.28	118.30
1	B	214	ARG	CD-NE-CZ	7.75	134.46	123.60
1	B	253	ASP	CB-CG-OD1	7.73	125.25	118.30
1	C	253	ASP	OD1-CG-OD2	-7.61	108.83	123.30
1	B	63	PHE	O-C-N	-7.61	110.52	122.70
1	A	247	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	C	98	GLU	OE1-CD-OE2	-7.59	114.20	123.30
1	D	274	ASP	CB-CG-OD2	7.56	125.10	118.30
1	B	123	ASP	CB-CG-OD2	7.48	125.03	118.30
1	B	210	ARG	NH1-CZ-NH2	-7.48	111.18	119.40
1	B	183	LEU	CB-CG-CD1	7.47	123.70	111.00
1	B	62	ASP	C-N-CA	7.42	140.25	121.70
1	B	242	GLU	OE1-CD-OE2	-7.40	114.42	123.30
1	D	124	GLU	OE1-CD-OE2	-7.40	114.42	123.30
1	C	99	ARG	NH1-CZ-NH2	-7.38	111.28	119.40
1	B	91	LYS	CD-CE-NZ	7.36	128.64	111.70
1	B	217	ASP	CB-CG-OD2	7.32	124.89	118.30
1	B	63	PHE	CA-C-N	7.31	133.28	117.20
1	B	183	LEU	CB-CG-CD2	7.28	123.38	111.00
1	D	67	TYR	CB-CG-CD2	-7.24	116.66	121.00
1	B	191	ASP	OD1-CG-OD2	-7.24	109.55	123.30
1	D	218	ARG	CG-CD-NE	-7.24	96.60	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	72	ASP	CB-CG-OD2	7.14	124.72	118.30
1	B	274	ASP	CB-CG-OD2	7.10	124.69	118.30
1	C	298	LEU	CB-CG-CD2	7.07	123.01	111.00
1	A	268	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	C	75	ASP	CB-CG-OD2	7.04	124.63	118.30
1	B	71	GLU	OE1-CD-OE2	-7.03	114.87	123.30
1	A	117	LEU	CB-CG-CD1	-7.01	99.08	111.00
1	B	274	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	164	GLU	OE1-CD-OE2	-6.99	114.91	123.30
1	B	74	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	C	67	TYR	N-CA-CB	-6.96	98.07	110.60
1	B	247	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	263	ASP	CB-CG-OD2	6.94	124.54	118.30
1	C	214	ARG	CD-NE-CZ	6.92	133.29	123.60
1	B	119	LEU	CD1-CG-CD2	-6.89	89.83	110.50
1	B	191	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	66	TYR	CB-CA-C	-6.88	96.64	110.40
1	C	74	ARG	CD-NE-CZ	6.88	133.24	123.60
1	A	277	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	139	MET	CG-SD-CE	6.85	111.17	100.20
1	C	239	PHE	CZ-CE2-CD2	6.85	128.32	120.10
1	C	183	LEU	CD1-CG-CD2	-6.83	90.00	110.50
1	C	103	ARG	CD-NE-CZ	6.82	133.15	123.60
1	B	239	PHE	CB-CG-CD1	6.82	125.57	120.80
1	B	62	ASP	CA-C-O	-6.81	105.80	120.10
1	C	63	PHE	O-C-N	-6.80	111.82	122.70
1	C	261	LEU	CD1-CG-CD2	-6.78	90.15	110.50
1	C	242	GLU	OE1-CD-OE2	-6.76	115.19	123.30
1	A	191	ASP	OD1-CG-OD2	-6.75	110.47	123.30
1	B	201	ASP	OD1-CG-OD2	-6.72	110.52	123.30
1	B	133	VAL	CB-CA-C	-6.70	98.66	111.40
1	C	218	ARG	CG-CD-NE	-6.69	97.75	111.80
1	A	259	GLU	OE1-CD-OE2	-6.69	115.27	123.30
1	A	115	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	247	ARG	CG-CD-NE	-6.65	97.84	111.80
1	A	253	ASP	OD1-CG-OD2	-6.64	110.69	123.30
1	B	219	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	B	274	ASP	OD1-CG-OD2	-6.63	110.70	123.30
1	C	253	ASP	CB-CG-OD1	6.63	124.26	118.30
1	C	132	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	C	218	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	D	201	ASP	OD1-CG-OD2	-6.57	110.81	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	218	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	190	LEU	CB-CG-CD2	-6.54	99.88	111.00
1	D	210	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	C	302	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	C	62	ASP	C-N-CA	-6.51	105.42	121.70
1	A	213	GLU	OE1-CD-OE2	-6.51	115.49	123.30
1	C	152	VAL	CG1-CB-CG2	-6.51	100.49	110.90
1	A	133	VAL	CB-CA-C	-6.50	99.05	111.40
1	C	66	TYR	CB-CG-CD1	-6.49	117.10	121.00
1	C	71	GLU	CA-CB-CG	6.49	127.68	113.40
1	B	174	GLU	CA-CB-CG	6.48	127.66	113.40
1	D	137	ASP	OD1-CG-OD2	-6.47	111.01	123.30
1	D	177	ASP	CB-CA-C	-6.44	97.52	110.40
1	C	219	ARG	NH1-CZ-NH2	-6.44	112.32	119.40
1	D	224	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	274	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	208	ARG	NH1-CZ-NH2	-6.38	112.38	119.40
1	B	64	SER	N-CA-C	-6.37	93.81	111.00
1	B	266	ASP	OD1-CG-OD2	-6.35	111.23	123.30
1	A	76	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	B	280	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	C	239	PHE	CB-CG-CD2	6.33	125.23	120.80
1	B	271	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	A	176	GLY	O-C-N	-6.31	112.60	122.70
1	A	197	LEU	CA-CB-CG	6.30	129.80	115.30
1	C	116	GLU	OE1-CD-OE2	-6.30	115.74	123.30
1	D	251	SER	CB-CA-C	-6.30	98.13	110.10
1	C	130	TYR	CD1-CE1-CZ	6.24	125.42	119.80
1	A	242	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	B	210	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	218	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	C	70	TYR	CD1-CE1-CZ	6.24	125.41	119.80
1	B	99	ARG	NE-CZ-NH2	6.23	123.41	120.30
1	D	76	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	228	GLU	OE1-CD-OE2	-6.22	115.84	123.30
1	B	115	ASP	CB-CG-OD2	6.15	123.84	118.30
1	B	71	GLU	CG-CD-OE2	6.14	130.59	118.30
1	B	76	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	280	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	66	TYR	N-CA-CB	-6.09	99.64	110.60
1	C	130	TYR	CB-CG-CD2	6.09	124.65	121.00
1	C	119	LEU	CD1-CG-CD2	-6.06	92.31	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	64	SER	N-CA-CB	-6.06	101.41	110.50
1	A	74	ARG	CG-CD-NE	-6.04	99.12	111.80
1	C	62	ASP	CB-CG-OD2	6.03	123.73	118.30
1	B	281	LEU	CB-CG-CD2	6.03	121.25	111.00
1	A	90	LYS	CD-CE-NZ	6.02	125.56	111.70
1	D	212	VAL	CG1-CB-CG2	-6.01	101.29	110.90
1	D	214	ARG	O-C-N	-6.01	113.09	122.70
1	B	218	ARG	CG-CD-NE	-6.00	99.19	111.80
1	C	70	TYR	CZ-CE2-CD2	5.99	125.19	119.80
1	D	286	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	263	ASP	CB-CG-OD2	5.97	123.68	118.30
1	C	70	TYR	CB-CG-CD2	5.96	124.58	121.00
1	C	62	ASP	N-CA-C	-5.95	94.94	111.00
1	D	214	ARG	CD-NE-CZ	5.94	131.91	123.60
1	D	137	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	65	THR	OG1-CB-CG2	-5.91	96.40	110.00
1	A	201	ASP	OD1-CG-OD2	-5.90	112.09	123.30
1	B	177	ASP	OD1-CG-OD2	-5.89	112.10	123.30
1	C	191	ASP	CB-CG-OD2	5.86	123.58	118.30
1	B	70	TYR	CB-CG-CD1	5.85	124.51	121.00
1	C	71	GLU	CB-CG-CD	-5.85	98.41	114.20
1	B	220	TYR	CZ-CE2-CD2	-5.85	114.54	119.80
1	B	239	PHE	CD1-CE1-CZ	5.84	127.11	120.10
1	A	204	GLU	OE1-CD-OE2	-5.84	116.29	123.30
1	C	75	ASP	OD1-CG-OD2	-5.83	112.22	123.30
1	C	76	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	C	298	LEU	CB-CG-CD1	5.83	120.90	111.00
1	B	62	ASP	N-CA-C	5.81	126.70	111.00
1	C	281	LEU	CD1-CG-CD2	-5.80	93.11	110.50
1	B	247	ARG	CG-CD-NE	-5.78	99.66	111.80
1	A	155	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	B	204	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	B	70	TYR	CD1-CE1-CZ	5.76	124.98	119.80
1	B	208	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	C	268	ARG	CD-NE-CZ	-5.75	115.55	123.60
1	C	271	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
1	C	72	ASP	OD1-CG-OD2	-5.72	112.44	123.30
1	C	201	ASP	OD1-CG-OD2	-5.70	112.47	123.30
1	A	271	ARG	NH1-CZ-NH2	-5.70	113.13	119.40
1	D	214	ARG	C-N-CA	-5.70	107.46	121.70
1	D	191	ASP	OD1-CG-OD2	-5.70	112.48	123.30
1	A	62	ASP	CB-CG-OD2	5.69	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	157	TYR	CD1-CE1-CZ	5.68	124.91	119.80
1	C	103	ARG	CG-CD-NE	-5.66	99.91	111.80
1	C	131	PHE	CB-CG-CD1	5.66	124.76	120.80
1	D	214	ARG	CA-C-N	5.64	129.62	117.20
1	D	274	ASP	OD1-CG-OD2	-5.64	112.58	123.30
1	A	228	GLU	OE1-CD-OE2	-5.59	116.60	123.30
1	B	124	GLU	CG-CD-OE2	5.58	129.47	118.30
1	C	88	LEU	CB-CG-CD2	5.58	120.48	111.00
1	A	226	LEU	CB-CG-CD2	5.58	120.48	111.00
1	D	133	VAL	CB-CA-C	-5.57	100.82	111.40
1	C	124	GLU	CG-CD-OE1	5.56	129.41	118.30
1	B	157	TYR	CB-CG-CD1	5.55	124.33	121.00
1	B	202	ARG	NE-CZ-NH2	5.55	123.07	120.30
1	D	75	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	285	VAL	CA-CB-CG2	5.52	119.18	110.90
1	A	217	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	158	VAL	CA-CB-CG2	-5.50	102.64	110.90
1	C	112	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	B	302	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	130	TYR	CD1-CE1-CZ	5.48	124.73	119.80
1	A	191	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	275	LEU	CB-CG-CD2	5.45	120.27	111.00
1	C	281	LEU	CB-CG-CD2	5.45	120.27	111.00
1	B	144	GLU	CG-CD-OE1	5.45	129.20	118.30
1	D	214	ARG	CG-CD-NE	-5.44	100.38	111.80
1	B	155	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	268	ARG	NH1-CZ-NH2	-5.42	113.44	119.40
1	C	88	LEU	CB-CG-CD1	-5.41	101.80	111.00
1	D	242	GLU	OE1-CD-OE2	-5.40	116.82	123.30
1	A	98	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	D	286	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	D	188	TYR	CD1-CE1-CZ	-5.39	114.95	119.80
1	B	208	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	B	64	SER	O-C-N	5.36	131.28	122.70
1	B	62	ASP	OD1-CG-OD2	-5.35	113.14	123.30
1	C	183	LEU	CB-CG-CD1	5.33	120.07	111.00
1	D	228	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	A	215	ASN	CB-CA-C	5.33	121.05	110.40
1	A	123	ASP	CB-CA-C	5.32	121.03	110.40
1	A	168	ARG	CB-CA-C	5.32	121.04	110.40
1	A	301	GLU	CB-CA-C	5.32	121.03	110.40
1	C	301	GLU	CB-CA-C	5.31	121.02	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	70	TYR	CD1-CG-CD2	-5.30	112.07	117.90
1	C	203	GLU	CA-CB-CG	-5.30	101.74	113.40
1	D	298	LEU	CB-CG-CD2	5.30	120.01	111.00
1	A	239	PHE	CZ-CE2-CD2	5.30	126.46	120.10
1	B	293	TYR	CD1-CE1-CZ	-5.29	115.03	119.80
1	C	75	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	67	TYR	N-CA-CB	-5.28	101.10	110.60
1	B	70	TYR	CD1-CG-CD2	-5.27	112.10	117.90
1	C	63	PHE	CB-CA-C	5.27	120.94	110.40
1	C	118	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	302	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	255	LEU	CB-CG-CD2	5.24	119.92	111.00
1	C	204	GLU	CG-CD-OE2	5.24	128.78	118.30
1	D	112	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	B	168	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	63	PHE	C-N-CA	-5.19	108.72	121.70
1	D	119	LEU	CB-CA-C	-5.19	100.33	110.20
1	C	121	VAL	CG1-CB-CG2	-5.19	102.60	110.90
1	B	62	ASP	CB-CA-C	5.18	120.75	110.40
1	D	212	VAL	CB-CA-C	-5.18	101.56	111.40
1	A	286	ARG	CG-CD-NE	-5.17	100.95	111.80
1	A	251	SER	N-CA-CB	-5.16	102.77	110.50
1	C	67	TYR	CB-CA-C	-5.15	100.10	110.40
1	B	62	ASP	CA-C-N	5.15	128.52	117.20
1	D	210	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	A	288	ARG	CG-CD-NE	-5.13	101.02	111.80
1	C	217	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	157	TYR	CB-CG-CD2	5.12	124.08	121.00
1	D	118	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	210	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	D	244	ARG	NE-CZ-NH1	-5.09	117.75	120.30
1	B	157	TYR	CZ-CE2-CD2	5.07	124.36	119.80
1	B	208	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	B	254	ASP	CB-CA-C	-5.06	100.28	110.40
1	B	139	MET	CG-SD-CE	5.05	108.28	100.20
1	B	298	LEU	CB-CG-CD2	5.03	119.56	111.00
1	B	87	LEU	CB-CG-CD2	-5.01	102.48	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	62	ASP	Peptide,Mainchain
1	B	63	PHE	Peptide,Mainchain
1	C	63	PHE	Peptide
1	D	63	PHE	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	2050	0	2055	82	1
1	B	2050	0	2054	89	2
1	C	2050	0	2054	74	3
1	D	2042	0	2051	62	3
2	A	232	0	0	22	2
2	B	215	0	0	25	1
2	C	199	0	0	30	1
2	D	235	0	0	21	1
All	All	9073	0	8214	262	7

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 16.

All (262) 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:139:MET:SD	1:D:139:MET:CE	2.03	1.46
1:B:104:MET:SD	1:B:104:MET:CE	2.06	1.40
1:B:175:LYS:HG2	2:B:492:HOH:O	1.12	1.26
1:B:175:LYS:HB2	2:B:506:HOH:O	1.13	1.26
1:D:175:LYS:HG2	2:D:526:HOH:O	1.34	1.22
1:A:173:SER:HB2	2:A:534:HOH:O	1.05	1.22
1:A:212:VAL:CG2	2:B:507:HOH:O	1.86	1.22
1:B:152:VAL:HG21	1:C:63:PHE:CE1	1.80	1.16
1:D:63:PHE:CE2	2:D:460:HOH:O	2.00	1.14
1:A:212:VAL:HB	2:B:507:HOH:O	1.51	1.11
1:A:176:GLY:O	1:A:177:ASP:HB3	1.40	1.11
1:D:286:ARG:HG2	2:D:446:HOH:O	1.49	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:LYS:CE	2:B:518:HOH:O	1.98	1.10
1:B:161:LYS:HD2	1:C:67:TYR:CE2	1.67	1.10
1:D:269:GLU:OE2	2:D:447:HOH:O	1.65	1.10
1:A:207:LYS:HG2	2:A:408:HOH:O	1.48	1.10
1:D:144:GLU:OE1	2:D:351:HOH:O	1.67	1.09
1:D:204:GLU:HG3	2:D:513:HOH:O	1.53	1.07
1:A:115:ASP:HB3	2:A:536:HOH:O	1.55	1.07
1:C:154:SER:HB3	2:C:499:HOH:O	1.61	1.01
1:C:164:GLU:OE2	2:C:458:HOH:O	1.78	1.01
1:B:62:ASP:N	1:B:67:TYR:CD2	2.27	1.01
1:C:67:TYR:HD1	2:C:412:HOH:O	1.44	1.00
1:B:143:LYS:HE3	2:B:518:HOH:O	1.59	1.00
1:B:161:LYS:CD	1:C:67:TYR:CE2	2.45	0.98
1:C:67:TYR:CD1	2:C:412:HOH:O	2.13	0.97
1:A:79:LYS:HB2	1:A:79:LYS:HZ2	1.29	0.95
1:C:66:TYR:CE1	2:C:415:HOH:O	2.19	0.95
1:B:152:VAL:CG2	1:C:63:PHE:CE1	2.50	0.95
1:D:153:LEU:H	1:D:199:ASN:HD21	1.15	0.94
1:A:79:LYS:NZ	1:A:79:LYS:CB	2.32	0.91
1:C:302:ARG:NE	2:C:369:HOH:O	1.95	0.90
1:D:63:PHE:CZ	2:D:460:HOH:O	2.17	0.90
2:A:510:HOH:O	1:B:64:SER:HB2	1.71	0.90
1:B:161:LYS:HD2	1:C:67:TYR:HE2	1.14	0.89
1:C:134:TYR:CB	2:C:494:HOH:O	2.21	0.89
1:A:207:LYS:NZ	2:A:344:HOH:O	2.00	0.88
1:C:62:ASP:N	2:C:464:HOH:O	2.06	0.87
1:B:152:VAL:HG11	1:C:63:PHE:CE1	2.11	0.86
1:B:174:GLU:OE1	2:B:399:HOH:O	1.92	0.85
1:A:79:LYS:HZ2	1:A:79:LYS:CB	1.88	0.85
1:C:190:LEU:HD23	2:C:401:HOH:O	1.76	0.85
1:D:220:TYR:CZ	1:D:224:ARG:HD3	2.12	0.85
1:C:199:ASN:H	1:C:199:ASN:HD22	1.26	0.84
1:D:224:ARG:NH1	2:D:530:HOH:O	2.08	0.84
1:C:115:ASP:OD2	2:C:491:HOH:O	1.94	0.84
1:C:134:TYR:HB3	2:C:494:HOH:O	1.75	0.83
1:A:176:GLY:O	1:A:177:ASP:CB	2.16	0.83
1:C:201:ASP:OD1	2:C:471:HOH:O	1.96	0.82
1:A:115:ASP:CB	2:A:536:HOH:O	2.18	0.82
1:D:199:ASN:HD22	1:D:199:ASN:H	1.28	0.82
1:A:63:PHE:HZ	1:D:152:VAL:HG12	1.46	0.80
1:B:81:LYS:HE2	1:B:88:LEU:HD12	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:ARG:HD2	2:D:530:HOH:O	1.84	0.78
1:B:152:VAL:CG1	1:C:63:PHE:HE1	1.96	0.78
1:A:63:PHE:HZ	1:D:152:VAL:CG1	1.96	0.78
1:C:220:TYR:CZ	1:C:224:ARG:HD2	2.19	0.78
1:B:161:LYS:NZ	1:C:67:TYR:CE1	2.50	0.77
1:B:175:LYS:CG	2:B:492:HOH:O	1.86	0.77
1:C:66:TYR:HE1	2:C:415:HOH:O	1.60	0.77
1:B:152:VAL:HG11	1:C:63:PHE:HE1	1.45	0.77
1:B:190:LEU:C	1:B:190:LEU:HD23	2.06	0.76
1:B:85:GLU:OE1	1:B:110:LYS:NZ	2.17	0.76
1:B:153:LEU:H	1:B:199:ASN:HD21	1.30	0.76
1:C:63:PHE:CA	1:C:64:SER:OG	2.34	0.75
1:C:100:LYS:O	2:C:346:HOH:O	2.05	0.75
1:D:144:GLU:OE1	2:D:424:HOH:O	2.05	0.74
1:A:211:GLU:OE2	2:A:530:HOH:O	2.05	0.74
1:A:212:VAL:CB	2:B:507:HOH:O	1.98	0.74
1:C:281:LEU:HD13	1:C:281:LEU:C	2.08	0.74
1:A:199:ASN:H	1:A:199:ASN:HD22	1.35	0.73
1:C:153:LEU:H	1:C:199:ASN:HD21	1.36	0.73
1:B:175:LYS:CG	2:B:506:HOH:O	2.25	0.73
1:A:159:ILE:HD13	1:B:62:ASP:HB2	1.71	0.72
1:B:139:MET:HE3	2:B:452:HOH:O	1.89	0.72
1:D:142:GLN:HE22	1:D:249:VAL:H	1.38	0.72
1:D:208:ARG:O	1:D:212:VAL:HG23	1.89	0.72
1:B:70:TYR:HE1	1:B:74:ARG:HH21	1.38	0.72
1:A:66:TYR:OH	2:A:359:HOH:O	2.01	0.71
1:A:145:GLU:OE1	2:A:475:HOH:O	2.08	0.71
1:B:161:LYS:CD	1:C:67:TYR:HE2	1.92	0.71
1:A:70:TYR:HE2	1:A:74:ARG:NH2	1.88	0.71
1:B:175:LYS:CB	2:B:506:HOH:O	1.87	0.71
1:C:161:LYS:HE3	2:C:500:HOH:O	1.90	0.70
1:C:168:ARG:HD3	1:C:169:TYR:CZ	2.26	0.70
1:A:79:LYS:HB2	1:A:79:LYS:NZ	2.01	0.70
1:A:63:PHE:CZ	1:D:152:VAL:HG12	2.27	0.70
1:B:166:PHE:CD2	1:B:174:GLU:HG2	2.25	0.70
1:A:79:LYS:NZ	1:A:79:LYS:HB3	2.07	0.70
1:B:152:VAL:CB	1:C:63:PHE:HE1	2.04	0.69
1:C:302:ARG:NH2	2:C:369:HOH:O	2.26	0.69
1:B:144:GLU:CD	2:B:460:HOH:O	2.32	0.68
1:C:71:GLU:OE2	2:C:490:HOH:O	2.11	0.68
1:C:217:ASP:OD1	2:C:503:HOH:O	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:H	1:A:199:ASN:HD21	1.38	0.68
1:A:212:VAL:HG21	2:B:507:HOH:O	1.63	0.68
1:B:161:LYS:NZ	2:B:463:HOH:O	2.26	0.67
1:A:79:LYS:HB3	1:A:79:LYS:HZ3	1.59	0.67
1:B:175:LYS:HG3	2:B:506:HOH:O	1.91	0.67
1:A:220:TYR:CZ	1:A:224:ARG:HD2	2.29	0.66
1:C:175:LYS:HG2	2:D:537:HOH:O	1.95	0.66
1:D:102:ILE:HB	1:D:107:ILE:HD12	1.76	0.66
1:B:63:PHE:CD2	1:B:67:TYR:HD1	2.14	0.65
1:B:178:LEU:HD12	2:B:456:HOH:O	1.95	0.65
1:C:63:PHE:N	1:C:64:SER:OG	2.29	0.65
1:A:82:ILE:CD1	1:D:198:LEU:HD21	2.27	0.65
1:A:74:ARG:NH1	1:D:161:LYS:HD2	2.11	0.65
1:A:85:GLU:OE1	1:A:110:LYS:NZ	2.29	0.65
1:A:115:ASP:CG	2:A:536:HOH:O	2.33	0.65
1:A:63:PHE:CZ	1:D:152:VAL:CG1	2.79	0.64
1:B:150:ALA:H	1:B:162:GLN:NE2	1.96	0.64
1:A:277:ARG:HB2	1:B:240:GLY:HA3	1.79	0.63
1:B:152:VAL:CB	1:C:63:PHE:CE1	2.81	0.63
2:B:463:HOH:O	1:C:67:TYR:CE1	2.50	0.63
1:A:79:LYS:CB	1:A:79:LYS:HZ3	2.11	0.63
1:C:204:GLU:HB2	2:C:497:HOH:O	1.99	0.63
1:B:142:GLN:HE22	1:B:249:VAL:H	1.47	0.62
1:C:63:PHE:HD2	1:C:67:TYR:HB2	1.63	0.62
1:D:204:GLU:CG	2:D:471:HOH:O	2.48	0.62
1:C:190:LEU:CD2	2:C:401:HOH:O	2.40	0.62
1:A:175:LYS:HE2	1:B:126:SER:OG	2.01	0.61
1:A:207:LYS:CG	2:A:408:HOH:O	2.25	0.61
1:C:85:GLU:OE1	1:C:110:LYS:NZ	2.28	0.61
1:A:150:ALA:H	1:A:162:GLN:NE2	1.98	0.61
1:D:268:ARG:HD3	2:D:529:HOH:O	1.99	0.61
1:A:82:ILE:HD11	1:D:198:LEU:HD21	1.83	0.60
1:B:63:PHE:CD2	1:B:67:TYR:CD1	2.89	0.60
1:D:88:LEU:HD13	2:D:536:HOH:O	2.00	0.60
1:B:143:LYS:HE2	2:B:518:HOH:O	1.84	0.60
1:A:199:ASN:HD22	1:A:199:ASN:N	2.00	0.59
1:C:147:PRO:HG3	2:C:458:HOH:O	2.03	0.59
1:D:204:GLU:CD	2:D:471:HOH:O	2.41	0.59
1:D:98:GLU:HG2	1:D:123:ASP:HA	1.85	0.59
1:A:150:ALA:H	1:A:162:GLN:HE21	1.48	0.59
1:C:281:LEU:HD13	1:C:281:LEU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLY:HA3	1:B:277:ARG:HB2	1.85	0.58
2:A:468:HOH:O	1:B:214:ARG:HG3	2.02	0.58
1:D:144:GLU:CD	2:D:424:HOH:O	2.41	0.58
1:A:70:TYR:CE2	1:A:74:ARG:NH2	2.70	0.58
1:B:143:LYS:CD	2:B:518:HOH:O	2.44	0.58
1:B:152:VAL:CG2	1:C:63:PHE:CZ	2.86	0.58
1:B:152:VAL:HG21	1:C:63:PHE:CZ	2.38	0.58
1:A:159:ILE:CD1	1:B:62:ASP:HB2	2.35	0.57
1:B:199:ASN:HD22	1:B:199:ASN:H	1.52	0.57
1:B:62:ASP:N	1:B:67:TYR:HD2	1.95	0.57
1:A:168:ARG:HD2	1:A:169:TYR:CE1	2.40	0.56
1:B:152:VAL:CG1	1:C:63:PHE:CE1	2.80	0.56
1:A:74:ARG:HH12	1:D:161:LYS:HD2	1.69	0.56
1:B:79:LYS:CB	1:B:79:LYS:NZ	2.69	0.55
1:D:286:ARG:CD	2:D:446:HOH:O	2.53	0.55
1:D:286:ARG:CG	2:D:446:HOH:O	2.25	0.55
1:C:199:ASN:HD22	1:C:199:ASN:N	1.96	0.55
1:B:63:PHE:HD2	1:B:67:TYR:HB2	1.72	0.55
1:B:164:GLU:CD	2:B:475:HOH:O	2.45	0.55
1:B:257:HIS:HD2	2:B:450:HOH:O	1.89	0.55
1:D:102:ILE:CG2	1:D:107:ILE:HD11	2.36	0.55
1:A:155:ASP:OD1	1:B:64:SER:CB	2.55	0.54
1:A:62:ASP:OD1	2:A:498:HOH:O	2.18	0.54
1:B:142:GLN:NE2	1:B:249:VAL:H	2.06	0.54
1:A:175:LYS:O	1:A:176:GLY:C	2.46	0.54
1:C:63:PHE:CD2	1:C:67:TYR:CG	2.96	0.54
1:B:96:ILE:HG21	1:B:119:LEU:HD22	1.90	0.53
1:D:96:ILE:HG21	1:D:119:LEU:HD22	1.90	0.53
2:A:510:HOH:O	1:B:65:THR:HG22	2.07	0.53
1:A:159:ILE:HD13	1:B:62:ASP:CB	2.38	0.53
1:B:164:GLU:OE2	2:B:475:HOH:O	2.19	0.53
1:C:286:ARG:NH1	2:C:368:HOH:O	2.41	0.53
1:C:225:ASN:HD21	1:C:229:ARG:HE	1.57	0.53
1:A:63:PHE:CD2	1:D:199:ASN:HB3	2.44	0.52
1:A:190:LEU:HD23	1:A:190:LEU:C	2.28	0.52
1:A:173:SER:CB	2:A:534:HOH:O	1.91	0.52
1:D:81:LYS:HE2	1:D:88:LEU:HD12	1.92	0.52
1:C:281:LEU:C	1:C:281:LEU:CD1	2.77	0.52
1:B:79:LYS:HZ2	1:B:79:LYS:HB2	1.75	0.51
1:A:302:ARG:CZ	2:A:535:HOH:O	2.58	0.51
1:B:129:THR:HG23	1:B:302:ARG:HD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:HG3	1:A:112:ARG:HH11	1.76	0.51
1:A:220:TYR:CE2	1:A:224:ARG:HD2	2.46	0.51
1:D:247:ARG:HD3	2:D:388:HOH:O	2.10	0.50
1:D:70:TYR:CE1	1:D:74:ARG:HD3	2.45	0.50
1:A:129:THR:HG23	1:A:302:ARG:HD2	1.93	0.50
1:C:220:TYR:CE2	1:C:224:ARG:HD2	2.46	0.50
1:A:168:ARG:HD3	1:A:169:TYR:CZ	2.47	0.50
1:D:199:ASN:HD22	1:D:199:ASN:N	2.02	0.50
1:A:62:ASP:N	2:A:421:HOH:O	2.44	0.49
1:C:99:ARG:HG2	1:D:212:VAL:HG12	1.94	0.49
1:A:63:PHE:CZ	1:D:152:VAL:HG11	2.47	0.49
1:B:190:LEU:HD23	1:B:190:LEU:O	2.12	0.49
1:D:224:ARG:CD	2:D:530:HOH:O	2.51	0.49
1:C:63:PHE:CD2	1:C:67:TYR:CD2	3.00	0.49
1:C:214:ARG:HG3	2:C:498:HOH:O	2.12	0.49
1:A:155:ASP:OD1	1:B:64:SER:HB2	2.13	0.49
1:A:213:GLU:OE1	1:A:219:ARG:NH2	2.46	0.49
1:C:277:ARG:HB2	1:D:240:GLY:HA3	1.94	0.49
1:A:266:ASP:HA	1:A:293:TYR:HA	1.95	0.48
1:B:129:THR:CG2	1:B:302:ARG:HD2	2.43	0.48
1:B:134:TYR:OH	1:B:288:ARG:HD3	2.14	0.48
1:C:240:GLY:HA3	1:D:277:ARG:HB2	1.96	0.48
1:C:79:LYS:CB	1:C:79:LYS:NZ	2.77	0.48
1:C:134:TYR:HB2	2:C:494:HOH:O	1.99	0.48
1:B:152:VAL:HG11	1:C:63:PHE:CD1	2.47	0.48
1:B:152:VAL:HB	1:C:63:PHE:HE1	1.78	0.48
1:B:208:ARG:O	1:B:212:VAL:HG12	2.14	0.48
1:D:65:THR:HG21	1:D:97:SER:HB2	1.95	0.48
1:D:102:ILE:CG2	1:D:107:ILE:CD1	2.91	0.48
1:B:71:GLU:O	1:B:75:ASP:HB2	2.14	0.47
1:A:70:TYR:HE2	1:A:74:ARG:HH21	1.58	0.47
1:B:79:LYS:NZ	1:B:79:LYS:HB2	2.30	0.47
1:B:187:LEU:HD22	1:B:206:VAL:HG22	1.95	0.47
1:A:155:ASP:OD1	1:B:64:SER:HB3	2.14	0.47
1:A:203:GLU:HG2	2:A:377:HOH:O	2.13	0.47
1:C:79:LYS:CB	1:C:79:LYS:HZ2	2.27	0.47
1:A:225:ASN:HD21	1:A:229:ARG:HE	1.63	0.47
1:A:184:ILE:CD1	1:A:219:ARG:HG2	2.45	0.47
1:D:156:GLU:OE2	2:D:352:HOH:O	2.20	0.46
1:B:143:LYS:HD3	2:B:518:HOH:O	2.12	0.46
1:C:210:ARG:NE	2:C:503:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:HG2	2:A:532:HOH:O	2.15	0.46
1:C:212:VAL:HG23	1:C:213:GLU:HG3	1.97	0.46
1:B:156:GLU:HG3	1:B:157:TYR:CE1	2.50	0.46
1:C:115:ASP:HA	2:C:494:HOH:O	2.15	0.46
1:B:190:LEU:C	1:B:190:LEU:CD2	2.82	0.45
1:B:247:ARG:NH2	1:B:260:TYR:OH	2.50	0.45
1:C:150:ALA:H	1:C:162:GLN:NE2	2.14	0.45
1:A:168:ARG:CB	1:A:168:ARG:HH11	2.30	0.45
1:A:63:PHE:CE2	1:D:199:ASN:HB3	2.52	0.45
1:A:100:LYS:O	2:A:321:HOH:O	2.20	0.44
1:A:123:ASP:OD2	1:B:235:THR:HG21	2.17	0.44
1:D:98:GLU:HG3	1:D:99:ARG:HD2	1.98	0.44
1:B:79:LYS:CB	1:B:79:LYS:HZ3	2.30	0.44
1:A:63:PHE:HZ	1:D:152:VAL:HG11	1.76	0.43
1:A:207:LYS:O	1:A:211:GLU:HG3	2.19	0.43
1:C:115:ASP:CG	2:C:491:HOH:O	2.51	0.43
1:D:142:GLN:NE2	1:D:249:VAL:H	2.10	0.43
1:A:236:GLY:O	1:A:237:PHE:C	2.57	0.43
1:B:245:VAL:HB	1:B:260:TYR:HB2	2.00	0.43
1:C:71:GLU:HB2	2:C:490:HOH:O	2.18	0.43
1:A:155:ASP:HB3	1:A:156:GLU:H	1.60	0.42
1:A:187:LEU:HD22	1:A:206:VAL:HG12	2.00	0.42
2:A:534:HOH:O	1:B:125:GLU:HB3	2.18	0.42
1:C:81:LYS:HE3	1:C:83:GLN:OE1	2.20	0.42
1:B:150:ALA:H	1:B:162:GLN:HE21	1.65	0.42
1:A:154:SER:O	1:A:155:ASP:CB	2.68	0.42
1:A:190:LEU:HD12	1:A:197:LEU:HD22	2.02	0.42
1:D:102:ILE:HG21	1:D:107:ILE:CD1	2.49	0.42
1:B:149:ILE:HB	1:B:162:GLN:HE21	1.85	0.42
1:D:178:LEU:N	1:D:178:LEU:HD12	2.34	0.42
1:D:214:ARG:HE	1:D:214:ARG:HB2	1.39	0.42
1:D:220:TYR:CE2	1:D:224:ARG:HD3	2.53	0.42
2:A:340:HOH:O	1:B:65:THR:CG2	2.67	0.41
1:C:126:SER:OG	1:D:175:LYS:HE3	2.19	0.41
1:A:63:PHE:CG	1:D:199:ASN:HB3	2.55	0.41
1:A:159:ILE:HD13	1:B:62:ASP:CG	2.41	0.41
1:D:102:ILE:CB	1:D:107:ILE:HD12	2.49	0.41
1:C:302:ARG:CZ	2:C:369:HOH:O	2.43	0.41
1:D:111:ALA:HB2	1:D:117:LEU:HD23	2.02	0.41
1:B:81:LYS:CE	1:B:88:LEU:HD12	2.42	0.41
1:B:204:GLU:HB2	2:B:413:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:VAL:HA	1:D:255:LEU:HD22	2.03	0.41
1:B:302:ARG:HH11	1:B:302:ARG:HD3	1.75	0.40
1:C:164:GLU:HB2	2:C:317:HOH:O	2.20	0.40
1:D:96:ILE:CG2	1:D:119:LEU:HD22	2.52	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:NE	1:C:203:GLU:OE1[3_545]	1.97	0.23
1:D:224:ARG:NH2	2:A:413:HOH:O[3_556]	1.99	0.21
1:A:203:GLU:OE2	1:D:224:ARG:NH2[3_546]	2.06	0.14
1:C:210:ARG:NH2	2:B:517:HOH:O[3_555]	2.07	0.13
1:D:269:GLU:OE2	2:A:529:HOH:O[3_556]	2.13	0.07
1:B:224:ARG:CD	1:C:203:GLU:OE1[3_545]	2.13	0.07
2:C:429:HOH:O	2:D:423:HOH:O[2_565]	2.18	0.02

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	242/305 (79%)	233 (96%)	6 (2%)	3 (1%)	13 7
1	B	242/305 (79%)	233 (96%)	9 (4%)	0	100 100
1	C	242/305 (79%)	234 (97%)	7 (3%)	1 (0%)	34 30
1	D	241/305 (79%)	234 (97%)	7 (3%)	0	100 100
All	All	967/1220 (79%)	934 (97%)	29 (3%)	4 (0%)	34 30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLY
1	A	177	ASP
1	A	155	ASP
1	C	155	ASP

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	222/273 (81%)	206 (93%)	16 (7%)	14 9
1	B	222/273 (81%)	202 (91%)	20 (9%)	9 6
1	C	222/273 (81%)	201 (90%)	21 (10%)	8 5
1	D	221/273 (81%)	203 (92%)	18 (8%)	11 7
All	All	887/1092 (81%)	812 (92%)	75 (8%)	10 6

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	74	ARG
1	A	79	LYS
1	A	99	ARG
1	A	100	LYS
1	A	123	ASP
1	A	143	LYS
1	A	168	ARG
1	A	177	ASP
1	A	197	LEU
1	A	199	ASN
1	A	207	LYS
1	A	261	LEU
1	A	295	LYS
1	A	301	GLU
1	A	302	ARG
1	B	62	ASP
1	B	63	PHE

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Mol	Chain	Res	Type
1	B	64	SER
1	B	65	THR
1	B	66	TYR
1	B	79	LYS
1	B	139	MET
1	B	143	LYS
1	B	152	VAL
1	B	174	GLU
1	B	183	LEU
1	B	192	LEU
1	B	196	ASN
1	B	199	ASN
1	B	207	LYS
1	B	212	VAL
1	B	214	ARG
1	B	295	LYS
1	B	298	LEU
1	B	302	ARG
1	C	62	ASP
1	C	66	TYR
1	C	71	GLU
1	C	74	ARG
1	C	79	LYS
1	C	82	ILE
1	C	139	MET
1	C	141	GLU
1	C	143	LYS
1	C	145	GLU
1	C	155	ASP
1	C	196	ASN
1	C	197	LEU
1	C	199	ASN
1	C	203	GLU
1	C	212	VAL
1	C	214	ARG
1	C	295	LYS
1	C	298	LEU
1	C	301	GLU
1	C	302	ARG
1	D	65	THR
1	D	66	TYR
1	D	79	LYS

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Mol	Chain	Res	Type
1	D	98	GLU
1	D	139	MET
1	D	142	GLN
1	D	145	GLU
1	D	156	GLU
1	D	162	GLN
1	D	183	LEU
1	D	196	ASN
1	D	199	ASN
1	D	203	GLU
1	D	204	GLU
1	D	214	ARG
1	D	235	THR
1	D	255	LEU
1	D	298	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	83	GLN
1	A	162	GLN
1	A	196	ASN
1	A	199	ASN
1	A	225	ASN
1	A	257	HIS
1	B	142	GLN
1	B	162	GLN
1	B	199	ASN
1	C	162	GLN
1	C	199	ASN
1	C	225	ASN
1	C	284	ASN
1	D	142	GLN
1	D	162	GLN
1	D	199	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	244/305 (80%)	0.04	7 (2%)	51	50	19, 27, 38, 50	0
1	B	244/305 (80%)	0.11	11 (4%)	33	32	19, 27, 38, 52	0
1	C	244/305 (80%)	0.06	9 (3%)	41	41	19, 27, 38, 50	0
1	D	243/305 (79%)	0.04	10 (4%)	37	36	18, 27, 38, 51	0
All	All	975/1220 (79%)	0.06	37 (3%)	40	39	18, 27, 38, 52	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	PHE	14.0
1	B	63	PHE	8.8
1	D	63	PHE	5.7
1	C	67	TYR	4.4
1	B	67	TYR	4.4
1	C	155	ASP	3.5
1	D	203	GLU	3.3
1	A	63	PHE	3.2
1	D	204	GLU	3.1
1	C	66	TYR	3.0
1	C	214	ARG	3.0
1	C	203	GLU	3.0
1	A	154	SER	3.0
1	B	203	GLU	2.9
1	D	79	LYS	2.8
1	D	177	ASP	2.8
1	A	168	ARG	2.8
1	D	67	TYR	2.8
1	A	79	LYS	2.5
1	B	79	LYS	2.5
1	A	203	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	66	TYR	2.5
1	B	201	ASP	2.5
1	A	212	VAL	2.4
1	B	62	ASP	2.4
1	C	79	LYS	2.4
1	D	233	VAL	2.4
1	B	64	SER	2.3
1	C	177	ASP	2.3
1	D	211	GLU	2.3
1	D	214	ARG	2.2
1	B	77	GLY	2.2
1	A	235	THR	2.2
1	C	145	GLU	2.2
1	B	214	ARG	2.1
1	D	74	ARG	2.1
1	B	121	VAL	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.