Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 10:32 AM EDT

PDB ID	:	3H66 / pdb_00003h66
Title	:	Catalytic domain of human Serine/Threonine Phosphatase 5 (PP5c) with two Zn2+ atoms
Authors	:	Bertini, I.; Calderone, V.; Fragai, M.; Luchinat, C.; Talluri, E.
Deposited on	:	2009-04-23
Resolution	:	2.59 Å(reported)

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

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

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

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

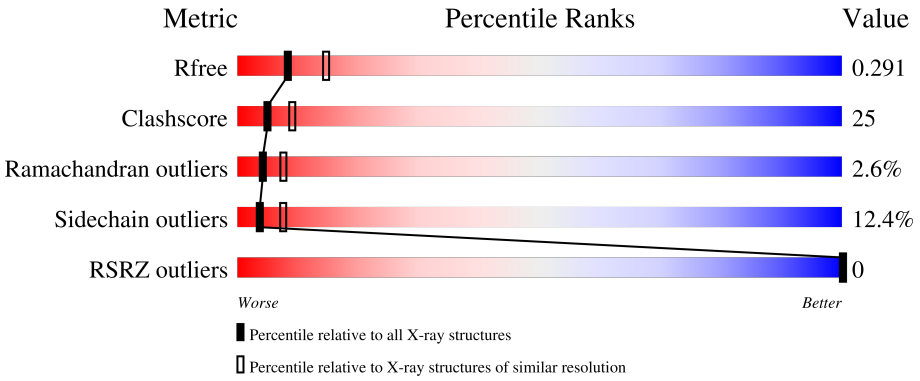
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.59 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (2.60-2.60)

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	315	17% 46% 30% 7%
1	B	315	21% 48% 26% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5116 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 Serine/threonine-protein phosphatase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2528	1615	425	473	15			
1	B	315	Total	C	N	O	S	0	0	0
			2528	1615	425	473	15			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is water.

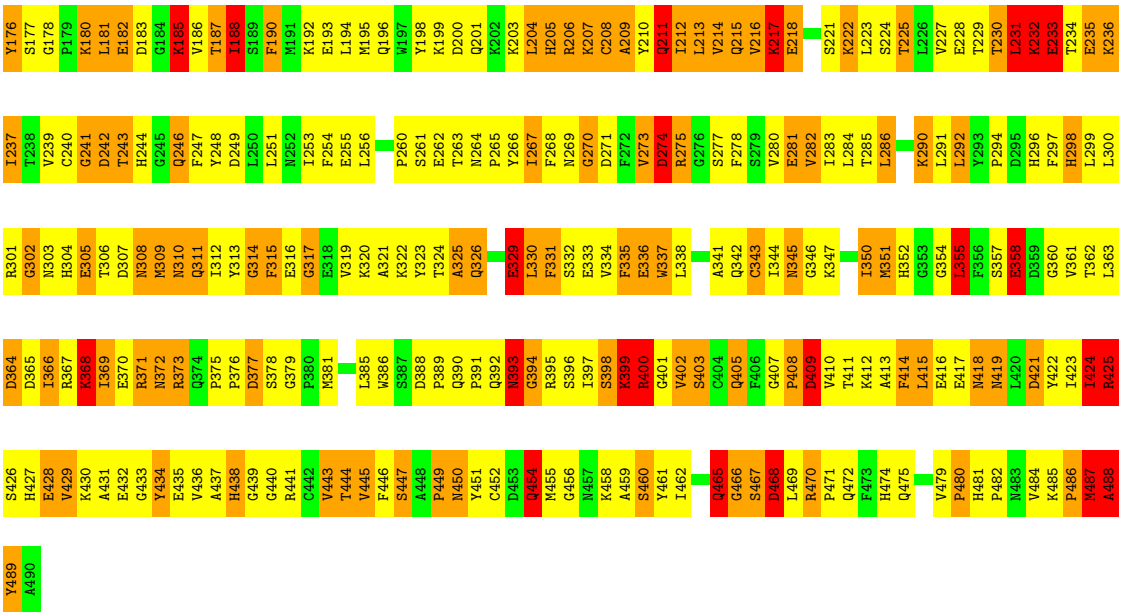
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	22	Total	O	0	0
			22	22		

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.

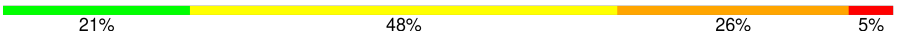
• Molecule 1: Serine/threonine-protein phosphatase 5

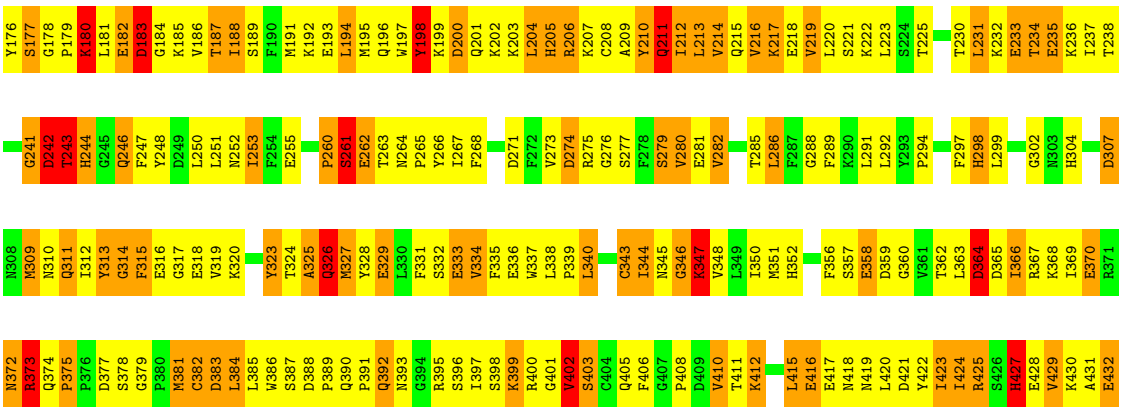
Chain A:



• Molecule 1: Serine/threonine-protein phosphatase 5

Chain B:






G433
Y434
E435
V436
A437
H438
R441
C442
V443
T444
V445
F446
S447
A448
P449
N450
Y451
C452
D453
Q454
M455
A459
S460
Y461
I462
H463
L464
Q465
G466
S467
D468
L469
R470
P471
Q472
F473
H474
Q475
F476
T477
A478
V479
P480
H481
P482
N483
V484
K485
P486
M487
A488
Y489
A490

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	154.25Å 41.68Å 106.09Å 90.00° 96.46° 90.00°	Depositor
Resolution (Å)	38.32 – 2.59 38.32 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.32-2.59) 92.4 (38.32-2.59)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.4.0067	Depositor
R, R_{free}	0.199 , 0.291 0.200 , 0.291	Depositor DCC
R_{free} test set	1821 reflections (9.23%)	wwPDB-VP
Wilson B-factor (Å^2)	4.4	Xtriage
Anisotropy	1.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 28.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5116	wwPDB-VP
Average B, all atoms (Å^2)	3.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	3.03	255/2592 (9.8%)	2.41	150/3506 (4.3%)
1	B	2.85	207/2592 (8.0%)	2.25	133/3506 (3.8%)
All	All	2.94	462/5184 (8.9%)	2.33	283/7012 (4.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (462) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	216	VAL	C-O	14.03	1.39	1.24
1	A	390	GLN	C-O	-13.07	1.10	1.24
1	A	381	MET	C-O	-12.99	1.07	1.24
1	A	214	VAL	CA-CB	12.84	1.73	1.54
1	A	296	HIS	CA-C	12.61	1.69	1.52
1	B	370	GLU	C-O	12.55	1.39	1.24
1	B	194	LEU	C-O	12.15	1.38	1.24
1	A	358	GLU	CG-CD	11.76	1.81	1.52
1	A	446	PHE	CA-C	-11.74	1.40	1.52
1	A	373	ARG	C-O	-11.64	1.10	1.23
1	A	251	LEU	C-O	-11.53	1.10	1.24
1	A	233	GLU	CG-CD	11.44	1.80	1.52
1	B	374	GLN	CA-C	11.40	1.66	1.53
1	B	219	VAL	CA-CB	11.37	1.67	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	358	GLU	CG-CD	11.18	1.79	1.52
1	A	325	ALA	C-O	11.11	1.36	1.24
1	B	429	VAL	C-O	-11.11	1.09	1.24
1	A	460	SER	C-O	11.06	1.34	1.24
1	A	410	VAL	N-CA	10.83	1.59	1.46
1	A	330	LEU	CA-C	10.81	1.66	1.52
1	A	429	VAL	C-O	-10.66	1.09	1.24
1	A	206	ARG	C-O	-10.57	1.10	1.24
1	B	410	VAL	C-O	10.48	1.36	1.24
1	A	244	HIS	N-CA	10.38	1.62	1.46
1	B	370	GLU	CA-C	10.25	1.65	1.52
1	A	267	ILE	N-CA	-10.19	1.34	1.46
1	A	430	LYS	C-O	-10.15	1.12	1.23
1	A	224	SER	C-O	-10.05	1.11	1.23
1	B	396	SER	N-CA	10.05	1.57	1.45
1	B	389	PRO	CA-C	9.71	1.64	1.52
1	B	274	ASP	CA-C	9.65	1.65	1.52
1	A	431	ALA	CA-CB	-9.56	1.37	1.53
1	A	377	ASP	N-CA	9.42	1.58	1.46
1	B	338	LEU	C-O	-9.40	1.12	1.24
1	B	434	TYR	CA-C	-9.40	1.41	1.52
1	B	210	TYR	CA-C	9.39	1.65	1.52
1	B	234	THR	CA-CB	9.30	1.67	1.54
1	A	193	GLU	N-CA	-9.09	1.34	1.46
1	A	417	GLU	CB-CG	-9.05	1.25	1.52
1	B	236	LYS	N-CA	8.98	1.57	1.45
1	B	180	LYS	C-O	8.88	1.35	1.23
1	B	282	VAL	CA-C	8.86	1.63	1.52
1	A	367	ARG	C-O	-8.85	1.13	1.24
1	B	461	TYR	CA-C	8.85	1.63	1.52
1	B	279	SER	C-O	8.79	1.34	1.24
1	A	347	LYS	C-O	-8.76	1.11	1.23
1	A	273	VAL	N-CA	-8.74	1.35	1.46
1	B	268	PHE	C-O	8.71	1.34	1.24
1	A	316	GLU	CA-C	-8.65	1.41	1.52
1	A	266	TYR	CA-C	8.50	1.63	1.52
1	B	385	LEU	CA-C	8.48	1.64	1.52
1	A	376	PRO	C-O	8.46	1.34	1.23
1	A	304	HIS	CA-C	8.45	1.64	1.52
1	B	241	GLY	N-CA	8.44	1.55	1.45
1	A	350	ILE	CA-CB	-8.44	1.43	1.54
1	A	395	ARG	C-O	-8.43	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	GLY	C-O	-8.41	1.12	1.24
1	A	375	PRO	CA-C	-8.41	1.47	1.51
1	A	225	THR	N-CA	-8.39	1.35	1.46
1	A	283	ILE	C-O	8.36	1.34	1.24
1	A	193	GLU	C-O	8.29	1.34	1.24
1	A	265	PRO	C-O	-8.29	1.13	1.23
1	A	399	LYS	CD-CE	8.28	1.77	1.52
1	A	481	HIS	C-O	8.27	1.34	1.24
1	A	326	GLN	CD-OE1	8.26	1.39	1.23
1	A	208	CYS	C-O	8.25	1.33	1.24
1	A	275	ARG	NE-CZ	8.21	1.42	1.33
1	B	391	PRO	C-O	8.21	1.34	1.24
1	A	458	LYS	N-CA	-8.19	1.35	1.45
1	B	483	ASN	CA-C	-8.18	1.43	1.53
1	B	479	VAL	CB-CG1	8.16	1.79	1.52
1	A	299	LEU	C-O	-8.14	1.14	1.24
1	B	244	HIS	N-CA	8.12	1.57	1.46
1	A	489	TYR	N-CA	8.11	1.56	1.46
1	A	409	ASP	CA-C	-8.10	1.42	1.52
1	B	206	ARG	N-CA	8.08	1.56	1.46
1	B	420	LEU	CA-C	8.06	1.63	1.52
1	A	330	LEU	CG-CD1	8.04	1.79	1.52
1	B	194	LEU	CG-CD2	8.02	1.79	1.52
1	B	194	LEU	CA-CB	-8.02	1.40	1.53
1	A	399	LYS	CE-NZ	8.00	1.73	1.49
1	A	255	GLU	CB-CG	-7.98	1.28	1.52
1	A	403	SER	C-O	-7.98	1.14	1.24
1	A	438	HIS	CA-C	-7.97	1.43	1.53
1	A	401	GLY	N-CA	7.94	1.57	1.45
1	B	208	CYS	N-CA	7.91	1.55	1.46
1	A	352	HIS	C-O	-7.83	1.14	1.23
1	A	443	VAL	CA-C	7.83	1.62	1.52
1	A	378	SER	CA-C	-7.81	1.43	1.52
1	B	446	PHE	CA-C	7.79	1.61	1.52
1	A	337	TRP	N-CA	7.78	1.56	1.45
1	B	255	GLU	CD-OE1	7.76	1.40	1.25
1	A	405	GLN	C-O	-7.73	1.14	1.24
1	A	468	ASP	C-O	7.69	1.33	1.24
1	A	290	LYS	C-O	7.68	1.33	1.24
1	B	237	ILE	CA-C	7.67	1.61	1.52
1	A	186	VAL	CA-C	-7.65	1.43	1.52
1	B	297	PHE	C-O	-7.62	1.14	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	464	LEU	CA-C	-7.60	1.43	1.52
1	A	358	GLU	CA-C	-7.58	1.43	1.52
1	A	341	ALA	CA-C	7.57	1.61	1.52
1	B	323	TYR	C-O	7.57	1.29	1.23
1	A	206	ARG	CG-CD	7.56	1.75	1.52
1	A	470	ARG	CZ-NH1	7.56	1.43	1.32
1	A	372	ASN	C-O	-7.55	1.14	1.24
1	B	447	SER	C-O	-7.54	1.14	1.24
1	A	335	PHE	C-O	7.51	1.32	1.24
1	B	233	GLU	CA-C	7.46	1.62	1.52
1	B	264	ASN	CA-CB	-7.46	1.44	1.53
1	A	441	ARG	NE-CZ	7.45	1.41	1.33
1	A	237	ILE	C-O	-7.45	1.16	1.24
1	A	209	ALA	C-O	-7.45	1.15	1.24
1	A	395	ARG	CZ-NH2	-7.44	1.23	1.33
1	B	307	ASP	N-CA	7.43	1.55	1.46
1	A	410	VAL	C-O	7.39	1.32	1.24
1	A	240	CYS	CA-C	-7.37	1.43	1.52
1	B	467	SER	N-CA	-7.35	1.38	1.46
1	A	429	VAL	CA-C	-7.35	1.44	1.53
1	A	371	ARG	N-CA	7.33	1.55	1.46
1	B	340	LEU	CA-C	7.26	1.62	1.52
1	B	264	ASN	N-CA	-7.25	1.39	1.46
1	B	326	GLN	C-O	-7.24	1.15	1.24
1	B	192	LYS	C-O	7.22	1.32	1.24
1	A	441	ARG	CD-NE	7.21	1.56	1.46
1	A	370	GLU	CG-CD	7.20	1.70	1.52
1	A	459	ALA	CA-CB	-7.20	1.42	1.53
1	A	435	GLU	N-CA	-7.19	1.36	1.45
1	A	190	PHE	C-O	7.18	1.32	1.24
1	B	431	ALA	C-O	-7.13	1.15	1.24
1	A	176	TYR	CA-C	7.13	1.68	1.52
1	B	288	GLY	C-O	7.12	1.32	1.23
1	B	214	VAL	CA-CB	7.12	1.63	1.54
1	A	440	GLY	C-O	-7.10	1.15	1.24
1	A	480	PRO	N-CA	7.10	1.55	1.47
1	A	270	GLY	C-O	-7.10	1.14	1.23
1	A	253	ILE	N-CA	7.05	1.54	1.46
1	B	275	ARG	CZ-NH1	7.03	1.42	1.32
1	A	264	ASN	C-N	7.03	1.41	1.33
1	A	195	MET	C-O	7.02	1.32	1.24
1	A	269	ASN	CA-C	7.00	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	ASP	CA-CB	-7.00	1.42	1.53
1	B	395	ARG	CA-C	-6.98	1.44	1.52
1	B	378	SER	N-CA	-6.98	1.38	1.46
1	B	196	GLN	C-O	6.96	1.32	1.24
1	B	391	PRO	CA-C	6.96	1.61	1.52
1	A	428	GLU	CA-C	6.96	1.61	1.52
1	A	304	HIS	N-CA	6.95	1.55	1.46
1	A	284	LEU	N-CA	-6.94	1.37	1.46
1	B	356	PHE	N-CA	6.94	1.54	1.45
1	A	386	TRP	CA-C	6.90	1.61	1.52
1	B	459	ALA	C-O	-6.85	1.15	1.23
1	A	331	PHE	C-O	-6.85	1.16	1.24
1	B	344	ILE	CA-C	6.84	1.60	1.52
1	B	378	SER	CA-C	6.83	1.60	1.52
1	A	417	GLU	CG-CD	-6.79	1.35	1.52
1	B	221	SER	C-O	-6.78	1.15	1.24
1	A	337	TRP	C-O	-6.78	1.15	1.24
1	A	321	ALA	CA-CB	6.78	1.64	1.53
1	A	370	GLU	C-O	6.77	1.32	1.23
1	B	244	HIS	C-O	-6.76	1.15	1.23
1	B	280	VAL	C-O	6.76	1.31	1.24
1	B	206	ARG	NE-CZ	6.75	1.40	1.33
1	B	316	GLU	CA-C	-6.74	1.44	1.52
1	A	480	PRO	CA-C	6.71	1.61	1.52
1	A	308	ASN	CA-CB	-6.69	1.42	1.53
1	A	261	SER	CA-C	-6.69	1.44	1.52
1	B	358	GLU	CD-OE1	6.69	1.38	1.25
1	A	268	PHE	CE1-CZ	-6.68	1.18	1.38
1	A	255	GLU	CA-CB	-6.68	1.42	1.53
1	A	180	LYS	CD-CE	6.67	1.72	1.52
1	A	216	VAL	C-O	6.65	1.31	1.24
1	A	228	GLU	C-O	-6.64	1.16	1.24
1	A	264	ASN	N-CA	-6.64	1.39	1.46
1	A	370	GLU	CD-OE2	6.64	1.38	1.25
1	B	250	LEU	CA-CB	-6.63	1.42	1.53
1	A	336	GLU	C-O	6.63	1.32	1.24
1	B	455	MET	C-O	-6.62	1.15	1.24
1	A	211	GLN	C-O	-6.62	1.16	1.24
1	B	424	ILE	C-O	6.62	1.30	1.24
1	B	191	MET	C-O	6.61	1.31	1.24
1	B	297	PHE	N-CA	-6.58	1.38	1.46
1	B	223	LEU	CA-CB	-6.57	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	415	LEU	CA-C	6.55	1.61	1.52
1	A	180	LYS	N-CA	6.54	1.53	1.46
1	B	375	PRO	C-O	6.54	1.30	1.25
1	B	415	LEU	CA-CB	-6.54	1.43	1.53
1	A	322	LYS	CA-C	6.53	1.61	1.52
1	B	470	ARG	CB-CG	6.52	1.72	1.52
1	B	374	GLN	C-N	6.50	1.39	1.33
1	A	292	LEU	C-O	-6.50	1.16	1.24
1	A	201	GLN	C-O	-6.49	1.13	1.24
1	A	216	VAL	CA-C	6.48	1.61	1.52
1	A	467	SER	C-O	6.48	1.32	1.24
1	B	441	ARG	NE-CZ	6.47	1.40	1.33
1	A	262	GLU	CD-OE1	6.47	1.37	1.25
1	B	253	ILE	CA-CB	-6.42	1.47	1.54
1	B	180	LYS	CE-NZ	6.41	1.68	1.49
1	A	487	MET	SD-CE	6.40	1.95	1.79
1	A	345	ASN	CG-OD1	-6.39	1.11	1.23
1	A	484	VAL	CA-CB	-6.39	1.46	1.54
1	B	179	PRO	C-O	-6.39	1.17	1.23
1	A	465	GLN	CD-NE2	6.35	1.46	1.33
1	B	356	PHE	C-O	6.34	1.31	1.23
1	B	331	PHE	C-O	6.33	1.31	1.24
1	A	377	ASP	C-O	-6.33	1.16	1.24
1	A	425	ARG	C-O	6.32	1.31	1.23
1	A	470	ARG	CZ-NH2	6.30	1.41	1.33
1	A	241	GLY	C-O	-6.29	1.15	1.23
1	B	320	LYS	C-O	6.28	1.31	1.24
1	A	291	LEU	C-O	6.28	1.31	1.24
1	B	260	PRO	C-O	-6.28	1.15	1.23
1	A	465	GLN	CA-C	-6.28	1.45	1.52
1	B	313	TYR	C-O	6.27	1.32	1.24
1	A	187	THR	CA-CB	6.26	1.65	1.54
1	B	216	VAL	CB-CG1	-6.26	1.31	1.52
1	A	424	ILE	C-O	-6.26	1.17	1.24
1	A	421	ASP	CA-C	-6.26	1.44	1.52
1	B	216	VAL	CA-C	6.25	1.60	1.52
1	A	319	VAL	N-CA	-6.24	1.39	1.46
1	B	187	THR	CA-C	-6.23	1.44	1.52
1	A	428	GLU	C-O	6.22	1.31	1.24
1	B	192	LYS	CA-C	6.22	1.60	1.52
1	B	241	GLY	C-O	6.21	1.29	1.23
1	A	237	ILE	CG1-CD1	-6.19	1.27	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	364	ASP	C-O	-6.18	1.16	1.24
1	B	282	VAL	N-CA	-6.17	1.39	1.46
1	A	449	PRO	CA-CB	6.17	1.62	1.53
1	B	200	ASP	CA-C	-6.15	1.42	1.52
1	A	185	LYS	CG-CD	6.14	1.70	1.52
1	B	441	ARG	CZ-NH1	6.14	1.41	1.32
1	A	200	ASP	C-O	-6.13	1.15	1.24
1	A	426	SER	C-O	-6.12	1.16	1.24
1	A	432	GLU	N-CA	6.12	1.54	1.46
1	B	399	LYS	CA-CB	6.10	1.63	1.53
1	B	280	VAL	CA-C	6.09	1.60	1.52
1	A	326	GLN	CD-NE2	6.09	1.46	1.33
1	A	274	ASP	CA-CB	-6.09	1.43	1.53
1	A	456	GLY	N-CA	-6.08	1.35	1.45
1	A	308	ASN	N-CA	-6.06	1.38	1.46
1	A	239	VAL	CA-C	6.05	1.60	1.52
1	A	454	GLN	C-O	6.05	1.31	1.24
1	A	254	PHE	C-O	6.04	1.31	1.24
1	B	264	ASN	CG-OD1	6.03	1.35	1.23
1	B	399	LYS	CG-CD	6.03	1.70	1.52
1	B	288	GLY	CA-C	6.02	1.58	1.51
1	B	382	CYS	C-O	6.02	1.31	1.24
1	B	312	ILE	CA-CB	6.01	1.62	1.54
1	B	217	LYS	CD-CE	6.00	1.70	1.52
1	A	355	LEU	CG-CD2	-6.00	1.32	1.52
1	A	249	ASP	C-O	-5.99	1.16	1.24
1	A	431	ALA	C-O	-5.98	1.16	1.24
1	A	434	TYR	C-O	-5.97	1.16	1.23
1	B	442	CYS	N-CA	5.97	1.53	1.46
1	B	218	GLU	CD-OE2	5.97	1.36	1.25
1	B	339	PRO	CA-C	5.97	1.59	1.52
1	A	419	ASN	C-O	-5.96	1.15	1.23
1	B	282	VAL	C-O	5.96	1.30	1.24
1	A	402	VAL	C-O	-5.96	1.16	1.23
1	A	449	PRO	C-O	-5.96	1.16	1.23
1	A	211	GLN	CD-OE1	5.95	1.34	1.23
1	B	218	GLU	CG-CD	5.95	1.67	1.52
1	B	299	LEU	C-O	-5.94	1.16	1.24
1	A	409	ASP	N-CA	-5.94	1.39	1.46
1	A	305	GLU	C-O	5.93	1.31	1.24
1	A	485	LYS	C-N	5.93	1.41	1.33
1	A	433	GLY	C-O	-5.93	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	267	ILE	CA-CB	5.92	1.61	1.54
1	A	228	GLU	CA-C	-5.91	1.45	1.52
1	B	381	MET	C-O	-5.91	1.17	1.24
1	B	357	SER	CA-C	5.90	1.60	1.52
1	A	201	GLN	N-CA	5.90	1.53	1.46
1	B	446	PHE	N-CA	5.88	1.53	1.46
1	A	216	VAL	N-CA	-5.87	1.39	1.46
1	B	297	PHE	CG-CD1	5.87	1.51	1.38
1	A	375	PRO	C-O	5.86	1.29	1.25
1	B	286	LEU	N-CA	-5.83	1.39	1.46
1	B	315	PHE	CE2-CZ	5.83	1.56	1.38
1	A	181	LEU	C-O	-5.82	1.17	1.24
1	A	266	TYR	N-CA	5.82	1.53	1.46
1	A	397	ILE	CG1-CD1	-5.81	1.29	1.51
1	A	322	LYS	CG-CD	5.80	1.69	1.52
1	B	194	LEU	CB-CG	-5.80	1.41	1.53
1	A	247	PHE	CA-C	5.79	1.60	1.52
1	B	324	THR	CA-C	5.78	1.59	1.52
1	A	402	VAL	CA-C	5.78	1.59	1.52
1	A	294	PRO	CA-C	5.78	1.62	1.52
1	B	187	THR	CA-CB	5.78	1.64	1.53
1	A	180	LYS	CE-NZ	5.77	1.66	1.49
1	A	310	ASN	C-O	5.77	1.30	1.24
1	B	294	PRO	CA-C	5.77	1.60	1.52
1	B	277	SER	CA-C	-5.77	1.45	1.52
1	B	358	GLU	CD-OE2	5.76	1.36	1.25
1	A	330	LEU	CA-CB	5.76	1.62	1.53
1	B	475	GLN	N-CA	5.76	1.52	1.45
1	A	217	LYS	C-O	-5.75	1.16	1.24
1	A	204	LEU	N-CA	5.73	1.53	1.45
1	A	421	ASP	C-O	-5.72	1.17	1.24
1	B	242	ASP	C-O	5.72	1.30	1.23
1	B	416	GLU	N-CA	5.72	1.53	1.46
1	A	486	PRO	C-O	5.71	1.30	1.23
1	A	311	GLN	N-CA	5.71	1.53	1.46
1	A	444	THR	CB-CG2	-5.71	1.33	1.52
1	B	196	GLN	CD-OE1	5.71	1.34	1.23
1	A	266	TYR	CB-CG	-5.70	1.39	1.51
1	A	185	LYS	CD-CE	5.70	1.69	1.52
1	A	223	LEU	N-CA	-5.69	1.39	1.46
1	B	471	PRO	N-CA	5.69	1.54	1.47
1	A	308	ASN	CB-CG	-5.69	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	486	PRO	N-CA	-5.68	1.40	1.47
1	A	470	ARG	CA-C	-5.68	1.45	1.52
1	B	247	PHE	C-O	5.68	1.30	1.24
1	B	289	PHE	CA-CB	-5.67	1.44	1.53
1	B	206	ARG	CZ-NH1	5.67	1.40	1.32
1	A	391	PRO	C-O	5.66	1.31	1.24
1	A	417	GLU	CA-C	-5.66	1.45	1.52
1	A	311	GLN	CG-CD	5.65	1.66	1.52
1	A	450	ASN	CG-OD1	5.65	1.34	1.23
1	A	408	PRO	C-O	-5.65	1.17	1.24
1	A	281	GLU	CA-C	-5.64	1.45	1.52
1	B	421	ASP	CA-C	-5.63	1.45	1.52
1	B	480	PRO	CG-CD	5.63	1.69	1.50
1	B	468	ASP	CB-CG	5.62	1.66	1.52
1	A	199	LYS	CA-CB	-5.62	1.44	1.53
1	B	338	LEU	CA-C	-5.62	1.47	1.53
1	A	216	VAL	CA-CB	5.61	1.61	1.54
1	A	351	MET	CA-C	-5.61	1.45	1.52
1	A	273	VAL	CA-C	-5.61	1.45	1.53
1	B	262	GLU	C-O	5.60	1.31	1.24
1	B	479	VAL	CA-CB	-5.60	1.47	1.54
1	A	240	CYS	C-O	5.59	1.30	1.23
1	A	255	GLU	N-CA	-5.59	1.39	1.46
1	B	435	GLU	C-O	5.58	1.31	1.23
1	A	351	MET	N-CA	-5.58	1.38	1.46
1	A	268	PHE	N-CA	5.57	1.53	1.46
1	A	270	GLY	C-N	-5.57	1.26	1.33
1	A	309	MET	SD-CE	5.56	1.93	1.79
1	A	254	PHE	CE2-CZ	5.55	1.55	1.38
1	B	220	LEU	CA-C	5.54	1.60	1.52
1	B	302	GLY	C-O	5.54	1.32	1.23
1	A	263	THR	CA-C	-5.54	1.46	1.52
1	B	359	ASP	C-O	5.53	1.31	1.23
1	A	260	PRO	CA-C	-5.53	1.45	1.52
1	B	422	TYR	CD1-CE1	5.53	1.55	1.38
1	B	473	PHE	CA-C	-5.52	1.46	1.52
1	B	332	SER	C-N	-5.50	1.25	1.33
1	A	488	ALA	CA-CB	5.50	1.62	1.53
1	B	428	GLU	CD-OE1	5.50	1.35	1.25
1	B	177	SER	C-O	5.50	1.31	1.24
1	B	373	ARG	CA-C	5.49	1.59	1.52
1	A	230	THR	CA-C	-5.49	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	PRO	N-CA	5.49	1.54	1.47
1	B	188	ILE	CA-CB	5.48	1.61	1.54
1	A	484	VAL	N-CA	-5.46	1.39	1.46
1	A	196	GLN	CB-CG	5.46	1.68	1.52
1	B	210	TYR	C-O	5.46	1.30	1.24
1	A	315	PHE	CG-CD1	5.46	1.50	1.38
1	B	369	ILE	CA-C	5.46	1.58	1.52
1	A	300	LEU	CA-C	-5.46	1.46	1.52
1	B	238	THR	C-O	-5.44	1.17	1.23
1	A	361	VAL	C-O	5.43	1.30	1.24
1	A	450	ASN	CA-CB	5.43	1.62	1.53
1	A	178	GLY	C-O	-5.42	1.16	1.24
1	A	294	PRO	N-CA	5.42	1.54	1.47
1	A	390	GLN	CD-OE1	5.41	1.33	1.23
1	B	347	LYS	N-CA	5.41	1.53	1.46
1	A	369	ILE	CA-CB	-5.39	1.45	1.53
1	A	485	LYS	CB-CG	5.39	1.68	1.52
1	A	369	ILE	N-CA	5.38	1.53	1.46
1	A	243	THR	CA-CB	-5.38	1.45	1.54
1	B	441	ARG	C-O	5.37	1.31	1.24
1	A	303	ASN	C-O	5.37	1.31	1.24
1	A	265	PRO	CA-C	-5.36	1.46	1.52
1	B	324	THR	CA-CB	-5.35	1.44	1.53
1	B	412	LYS	CD-CE	5.35	1.68	1.52
1	A	308	ASN	C-O	5.35	1.30	1.24
1	B	357	SER	C-O	-5.35	1.17	1.24
1	B	218	GLU	CD-OE1	5.34	1.35	1.25
1	A	336	GLU	N-CA	-5.33	1.39	1.46
1	B	403	SER	C-O	-5.33	1.17	1.24
1	B	263	THR	CB-CG2	5.32	1.70	1.52
1	B	399	LYS	CB-CG	5.31	1.68	1.52
1	A	393	ASN	N-CA	5.31	1.53	1.46
1	B	325	ALA	C-O	5.30	1.30	1.24
1	A	306	THR	N-CA	5.30	1.52	1.46
1	B	198	TYR	CE1-CZ	5.29	1.50	1.38
1	A	344	ILE	CG1-CD1	-5.29	1.31	1.51
1	B	448	ALA	CA-C	5.29	1.59	1.52
1	A	281	GLU	C-O	5.29	1.30	1.24
1	A	213	LEU	CG-CD2	-5.27	1.35	1.52
1	A	430	LYS	CA-C	-5.27	1.46	1.52
1	B	241	GLY	CA-C	5.26	1.58	1.51
1	A	217	LYS	CE-NZ	5.26	1.65	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	CYS	C-O	-5.26	1.17	1.24
1	A	401	GLY	C-O	-5.25	1.16	1.24
1	B	194	LEU	CG-CD1	-5.24	1.35	1.52
1	A	470	ARG	N-CA	-5.24	1.37	1.45
1	B	344	ILE	C-O	5.24	1.29	1.24
1	B	392	GLN	C-O	5.23	1.30	1.23
1	B	324	THR	N-CA	5.23	1.52	1.45
1	B	479	VAL	CB-CG2	-5.23	1.35	1.52
1	A	419	ASN	CG-ND2	5.22	1.44	1.33
1	B	461	TYR	C-O	5.22	1.30	1.23
1	B	211	GLN	CG-CD	5.21	1.65	1.52
1	A	299	LEU	CG-CD2	-5.21	1.35	1.52
1	B	375	PRO	CB-CG	5.20	1.75	1.49
1	B	311	GLN	N-CA	5.19	1.52	1.46
1	B	326	GLN	N-CA	-5.19	1.40	1.46
1	A	286	LEU	CA-C	5.18	1.60	1.52
1	A	445	VAL	CA-C	5.18	1.59	1.52
1	B	266	TYR	CZ-OH	5.18	1.49	1.38
1	A	236	LYS	C-O	5.18	1.30	1.23
1	A	472	GLN	CD-NE2	5.18	1.44	1.33
1	B	455	MET	CA-C	-5.18	1.45	1.52
1	A	251	LEU	CA-C	-5.18	1.46	1.52
1	A	425	ARG	CZ-NH1	5.17	1.40	1.32
1	A	368	LYS	CA-C	-5.17	1.45	1.52
1	A	298	HIS	CA-CB	-5.17	1.44	1.53
1	B	208	CYS	CB-SG	-5.17	1.64	1.81
1	B	255	GLU	CA-CB	-5.16	1.45	1.53
1	B	320	LYS	CE-NZ	5.16	1.64	1.49
1	B	251	LEU	C-O	-5.14	1.18	1.24
1	B	442	CYS	CB-SG	5.14	1.98	1.81
1	B	205	HIS	N-CA	5.14	1.52	1.45
1	B	334	VAL	CA-CB	-5.14	1.48	1.54
1	A	267	ILE	CG1-CD1	-5.13	1.31	1.51
1	B	246	GLN	C-O	5.13	1.29	1.23
1	A	332	SER	N-CA	-5.13	1.40	1.46
1	A	215	GLN	N-CA	-5.12	1.39	1.46
1	A	358	GLU	CD-OE2	5.12	1.35	1.25
1	B	219	VAL	CA-C	-5.11	1.46	1.52
1	B	450	ASN	CA-C	5.11	1.59	1.52
1	A	218	GLU	N-CA	-5.10	1.40	1.46
1	B	291	LEU	N-CA	5.10	1.52	1.46
1	A	402	VAL	CA-CB	5.10	1.62	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	477	THR	N-CA	-5.10	1.38	1.46
1	A	212	ILE	CA-CB	-5.08	1.48	1.54
1	B	230	THR	C-O	-5.08	1.18	1.24
1	B	289	PHE	C-O	-5.08	1.17	1.24
1	B	213	LEU	CG-CD1	5.07	1.69	1.52
1	B	196	GLN	CA-C	5.06	1.59	1.52
1	B	370	GLU	N-CA	-5.06	1.40	1.46
1	B	485	LYS	N-CA	5.06	1.52	1.45
1	A	322	LYS	CE-NZ	-5.06	1.34	1.49
1	A	424	ILE	N-CA	5.05	1.52	1.46
1	B	410	VAL	N-CA	5.05	1.52	1.46
1	A	347	LYS	CD-CE	5.05	1.67	1.52
1	A	285	THR	N-CA	5.05	1.52	1.46
1	A	342	GLN	N-CA	-5.05	1.39	1.46
1	B	346	GLY	C-O	5.05	1.30	1.24
1	B	436	VAL	CA-CB	-5.05	1.47	1.53
1	B	315	PHE	CG-CD1	5.04	1.49	1.38
1	B	378	SER	C-O	-5.04	1.17	1.23
1	A	290	LYS	CG-CD	-5.03	1.37	1.52
1	B	237	ILE	C-O	5.03	1.29	1.23
1	B	192	LYS	CE-NZ	5.03	1.64	1.49
1	B	242	ASP	N-CA	5.03	1.52	1.46
1	B	261	SER	C-O	5.02	1.30	1.24
1	B	482	PRO	C-O	5.02	1.30	1.23
1	B	212	ILE	CA-CB	-5.01	1.48	1.54
1	B	184	GLY	N-CA	5.01	1.52	1.45
1	B	343	CYS	N-CA	5.00	1.52	1.46
1	A	323	TYR	N-CA	-5.00	1.39	1.46

All (283) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	481	HIS	CA-C-N	-13.33	107.32	120.52
1	A	481	HIS	C-N-CA	-13.33	107.32	120.52
1	B	367	ARG	N-CA-C	-13.03	97.06	111.14
1	A	358	GLU	N-CA-C	-11.33	92.13	109.24
1	A	325	ALA	N-CA-C	-11.12	99.17	111.07
1	A	317	GLY	N-CA-C	-11.11	99.40	112.73
1	B	309	MET	N-CA-C	-11.00	99.37	111.36
1	A	319	VAL	N-CA-C	-10.53	101.16	110.74
1	A	375	PRO	CA-C-N	-10.38	110.25	120.21
1	A	375	PRO	C-N-CA	-10.38	110.25	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	346	GLY	N-CA-C	-10.01	98.98	114.10
1	A	329	GLU	N-CA-C	-9.92	99.73	112.23
1	A	366	ILE	N-CA-C	-9.85	101.14	111.58
1	A	446	PHE	CB-CA-C	-9.80	97.17	110.79
1	A	354	GLY	N-CA-C	9.76	124.11	110.74
1	A	192	LYS	N-CA-C	-9.54	100.74	111.71
1	A	329	GLU	CA-C-N	-9.53	108.06	120.44
1	A	329	GLU	C-N-CA	-9.53	108.06	120.44
1	A	399	LYS	N-CA-C	-9.38	101.76	113.01
1	B	316	GLU	N-CA-C	-9.23	100.33	111.69
1	A	365	ASP	N-CA-C	9.13	123.44	111.75
1	B	183	ASP	N-CA-C	-9.09	91.44	110.80
1	B	204	LEU	N-CA-C	-9.06	98.32	110.55
1	A	386	TRP	N-CA-C	9.05	125.22	113.18
1	B	378	SER	N-CA-CB	-9.01	97.58	111.46
1	A	394	GLY	N-CA-C	8.97	127.01	112.84
1	B	481	HIS	CA-C-N	-8.96	111.60	120.21
1	B	481	HIS	C-N-CA	-8.96	111.60	120.21
1	A	282	VAL	N-CA-CB	8.90	120.39	110.51
1	A	470	ARG	N-CA-C	-8.82	98.92	110.39
1	A	312	ILE	CB-CA-C	-8.81	102.84	111.30
1	B	243	THR	N-CA-C	-8.64	103.86	114.75
1	A	370	GLU	CB-CG-CD	8.50	127.05	112.60
1	A	244	HIS	CB-CA-C	-8.44	99.29	111.95
1	A	378	SER	N-CA-C	-8.41	94.18	107.73
1	A	203	LYS	CB-CG-CD	-8.41	91.96	111.30
1	A	400	ARG	NE-CZ-NH1	-8.36	113.14	121.50
1	B	386	TRP	N-CA-C	8.15	123.90	113.88
1	A	199	LYS	N-CA-C	-8.12	102.43	111.28
1	B	448	ALA	CA-C-N	8.10	128.05	120.03
1	B	448	ALA	C-N-CA	8.10	128.05	120.03
1	A	368	LYS	CD-CE-NZ	-7.99	86.34	111.90
1	A	309	MET	N-CA-C	-7.89	102.63	111.07
1	A	322	LYS	N-CA-C	-7.82	104.26	113.88
1	B	219	VAL	CB-CA-C	-7.79	102.07	111.81
1	A	377	ASP	CB-CA-C	-7.75	95.00	110.42
1	A	207	LYS	N-CA-C	-7.74	102.76	112.90
1	A	192	LYS	CA-C-N	-7.71	107.40	120.58
1	A	192	LYS	C-N-CA	-7.71	107.40	120.58
1	A	379	GLY	CA-C-N	7.71	127.25	119.24
1	A	379	GLY	C-N-CA	7.71	127.25	119.24
1	A	344	ILE	CB-CA-C	-7.67	99.88	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	333	GLU	N-CA-C	-7.64	101.83	112.45
1	A	450	ASN	N-CA-C	-7.60	100.97	111.30
1	A	367	ARG	NE-CZ-NH2	-7.55	112.40	119.20
1	B	201	GLN	N-CA-C	7.50	121.84	112.24
1	B	369	ILE	N-CA-C	7.49	119.05	108.93
1	A	206	ARG	CG-CD-NE	-7.42	95.68	112.00
1	A	177	SER	N-CA-C	-7.39	103.39	113.30
1	A	414	PHE	N-CA-C	7.35	120.22	111.33
1	B	236	LYS	CD-CE-NZ	-7.31	88.50	111.90
1	A	357	SER	O-C-N	-7.30	112.90	122.39
1	A	419	ASN	N-CA-C	7.30	121.58	112.24
1	A	247	PHE	N-CA-C	7.29	120.15	111.33
1	B	243	THR	CA-C-N	-7.29	112.47	122.82
1	B	243	THR	C-N-CA	-7.29	112.47	122.82
1	B	399	LYS	CB-CG-CD	7.26	128.01	111.30
1	B	385	LEU	CB-CG-CD2	-7.15	89.24	110.70
1	B	191	MET	CA-C-N	-7.14	110.16	120.29
1	B	191	MET	C-N-CA	-7.14	110.16	120.29
1	B	255	GLU	N-CA-C	7.12	120.45	111.69
1	A	439	GLY	CA-C-N	7.05	130.98	123.08
1	A	439	GLY	C-N-CA	7.05	130.98	123.08
1	A	185	LYS	N-CA-C	-7.05	97.81	108.46
1	A	277	SER	N-CA-C	6.97	121.39	113.02
1	B	344	ILE	CB-CA-C	-6.95	100.47	110.83
1	B	340	LEU	N-CA-C	6.91	121.46	112.89
1	A	396	SER	CA-CB-OG	6.89	124.89	111.10
1	B	262	GLU	CA-C-N	-6.88	111.72	122.67
1	B	262	GLU	C-N-CA	-6.88	111.72	122.67
1	A	410	VAL	N-CA-CB	6.87	118.14	110.51
1	A	260	PRO	N-CA-C	-6.86	101.12	111.41
1	B	276	GLY	N-CA-C	-6.86	103.36	112.82
1	A	413	ALA	N-CA-C	6.83	119.36	111.02
1	A	208	CYS	N-CA-C	-6.80	103.55	110.97
1	A	222	LYS	CA-C-N	-6.77	112.56	122.65
1	A	222	LYS	C-N-CA	-6.77	112.56	122.65
1	A	324	THR	CB-CA-C	-6.76	97.99	111.91
1	B	418	ASN	N-CA-C	-6.72	104.30	113.30
1	B	384	LEU	CB-CG-CD2	-6.70	90.61	110.70
1	B	399	LYS	N-CA-C	-6.67	103.22	111.75
1	B	193	GLU	N-CA-CB	6.63	120.56	110.28
1	A	446	PHE	CA-C-O	-6.60	111.11	120.15
1	B	400	ARG	NE-CZ-NH1	-6.56	114.94	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	442	CYS	N-CA-C	6.56	121.41	107.70
1	B	427	HIS	N-CA-CB	-6.56	99.41	110.49
1	B	343	CYS	CA-C-O	-6.55	113.29	120.36
1	B	348	VAL	N-CA-C	-6.53	98.71	108.12
1	B	255	GLU	CG-CD-OE2	-6.53	103.39	118.40
1	A	285	THR	CB-CA-C	-6.51	100.93	110.96
1	A	331	PHE	N-CA-C	-6.51	103.45	111.33
1	A	409	ASP	CA-C-O	-6.51	113.98	120.82
1	B	208	CYS	N-CA-C	-6.51	104.11	111.07
1	B	329	GLU	CA-C-N	-6.46	111.82	120.54
1	B	329	GLU	C-N-CA	-6.46	111.82	120.54
1	A	360	GLY	N-CA-C	-6.46	106.22	115.64
1	A	367	ARG	NE-CZ-NH1	6.45	127.95	121.50
1	A	439	GLY	N-CA-C	6.44	124.82	114.90
1	B	236	LYS	CA-CB-CG	-6.43	101.23	114.10
1	A	205	HIS	N-CA-C	-6.42	100.97	110.48
1	B	313	TYR	N-CA-C	6.40	121.14	112.88
1	B	265	PRO	CA-C-O	-6.39	113.64	121.31
1	A	351	MET	N-CA-C	-6.37	99.94	108.74
1	B	194	LEU	CB-CG-CD1	-6.35	91.66	110.70
1	A	216	VAL	N-CA-C	-6.33	104.68	110.82
1	A	203	LYS	N-CA-C	6.27	119.68	109.59
1	B	211	GLN	N-CA-C	-6.26	104.38	111.14
1	B	267	ILE	CB-CA-C	-6.16	101.51	110.63
1	A	240	CYS	N-CA-C	-6.16	99.77	109.50
1	A	251	LEU	N-CA-C	-6.15	104.49	111.14
1	B	233	GLU	CB-CA-C	6.15	122.65	110.42
1	A	470	ARG	CA-C-N	-6.14	113.36	119.99
1	A	470	ARG	C-N-CA	-6.14	113.36	119.99
1	A	266	TYR	CA-C-N	-6.13	115.59	123.19
1	A	266	TYR	C-N-CA	-6.13	115.59	123.19
1	B	182	GLU	N-CA-C	6.13	119.22	108.56
1	A	417	GLU	CB-CA-C	-6.12	98.92	110.67
1	A	400	ARG	NE-CZ-NH2	6.11	124.70	119.20
1	B	194	LEU	CA-C-N	-6.11	112.09	120.28
1	B	194	LEU	C-N-CA	-6.11	112.09	120.28
1	A	357	SER	CA-C-N	-6.10	112.32	122.21
1	A	357	SER	C-N-CA	-6.10	112.32	122.21
1	A	443	VAL	O-C-N	-6.09	116.47	122.93
1	B	432	GLU	CA-C-O	-6.09	112.06	119.43
1	A	395	ARG	CA-C-O	-6.05	113.70	120.66
1	A	302	GLY	N-CA-C	6.05	122.46	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	443	VAL	N-CA-C	6.03	116.86	108.89
1	B	478	ALA	CA-C-O	-6.03	113.98	120.92
1	B	297	PHE	O-C-N	-5.99	115.47	123.14
1	A	299	LEU	CA-C-O	-5.99	113.85	120.38
1	A	440	GLY	N-CA-C	-5.98	107.37	114.48
1	A	230	THR	CA-C-O	-5.97	113.91	120.24
1	B	199	LYS	CA-C-N	-5.97	111.03	122.61
1	B	199	LYS	C-N-CA	-5.97	111.03	122.61
1	A	316	GLU	N-CA-C	-5.95	104.38	111.69
1	B	267	ILE	CA-C-N	-5.93	114.69	123.11
1	B	267	ILE	C-N-CA	-5.93	114.69	123.11
1	A	371	ARG	N-CA-C	5.91	120.22	112.89
1	A	447	SER	N-CA-C	5.90	120.04	112.26
1	A	204	LEU	N-CA-C	-5.86	102.64	110.55
1	B	345	ASN	CA-C-N	5.80	130.87	120.77
1	B	345	ASN	C-N-CA	5.80	130.87	120.77
1	A	260	PRO	CA-C-O	-5.79	114.66	122.08
1	B	299	LEU	CA-C-N	-5.79	113.08	122.81
1	B	299	LEU	C-N-CA	-5.79	113.08	122.81
1	A	180	LYS	CD-CE-NZ	5.79	130.41	111.90
1	B	223	LEU	N-CA-C	5.78	119.51	110.32
1	B	244	HIS	N-CA-C	5.77	119.31	111.17
1	A	461	TYR	N-CA-C	-5.72	100.85	108.74
1	A	218	GLU	N-CA-C	5.71	117.37	111.03
1	A	418	ASN	CA-C-N	-5.71	114.12	122.40
1	A	418	ASN	C-N-CA	-5.71	114.12	122.40
1	A	232	LYS	CA-CB-CG	5.71	125.52	114.10
1	B	192	LYS	N-CA-C	-5.70	105.15	111.36
1	B	298	HIS	N-CA-C	5.70	118.76	109.59
1	B	285	THR	CA-C-O	5.70	126.80	120.82
1	B	454	GLN	CB-CG-CD	-5.69	102.92	112.60
1	B	374	GLN	CB-CA-C	5.69	117.63	109.26
1	A	267	ILE	CA-C-N	-5.69	115.03	123.11
1	A	267	ILE	C-N-CA	-5.69	115.03	123.11
1	A	347	LYS	CA-C-O	-5.68	112.40	120.07
1	A	233	GLU	CA-CB-CG	5.67	125.44	114.10
1	A	297	PHE	N-CA-C	-5.66	97.76	107.61
1	B	387	SER	N-CA-C	-5.66	102.39	110.59
1	A	267	ILE	CA-CB-CG1	5.66	120.02	110.40
1	B	212	ILE	CA-C-N	-5.65	112.94	120.79
1	B	212	ILE	C-N-CA	-5.65	112.94	120.79
1	A	234	THR	CB-CA-C	-5.64	100.07	109.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	431	ALA	N-CA-C	-5.61	105.16	111.28
1	B	399	LYS	O-C-N	-5.61	115.81	122.20
1	A	335	PHE	N-CA-C	-5.59	105.18	111.28
1	A	256	LEU	N-CA-C	-5.58	105.59	112.90
1	A	399	LYS	CA-C-N	-5.58	112.96	122.56
1	A	399	LYS	C-N-CA	-5.58	112.96	122.56
1	A	186	VAL	CB-CA-C	-5.57	103.94	111.63
1	A	466	GLY	N-CA-C	5.56	119.40	112.73
1	A	415	LEU	N-CA-CB	5.55	118.28	110.12
1	B	370	GLU	CA-C-O	5.55	126.88	120.60
1	A	314	GLY	CA-C-N	-5.55	112.77	120.38
1	A	314	GLY	C-N-CA	-5.55	112.77	120.38
1	B	454	GLN	CB-CA-C	-5.55	100.47	109.13
1	A	198	TYR	N-CA-C	-5.54	105.25	112.23
1	A	364	ASP	N-CA-C	5.53	122.58	110.80
1	B	178	GLY	CA-C-N	-5.53	114.02	119.99
1	B	178	GLY	C-N-CA	-5.53	114.02	119.99
1	B	324	THR	N-CA-C	5.53	117.38	109.14
1	B	189	SER	CA-CB-OG	-5.49	100.12	111.10
1	A	299	LEU	N-CA-C	5.48	117.89	109.07
1	B	432	GLU	CA-C-N	-5.47	114.88	122.86
1	B	432	GLU	C-N-CA	-5.47	114.88	122.86
1	B	383	ASP	N-CA-C	-5.46	105.23	111.07
1	A	489	TYR	N-CA-CB	5.46	118.56	110.49
1	B	441	ARG	CA-C-N	-5.46	115.09	122.95
1	B	441	ARG	C-N-CA	-5.46	115.09	122.95
1	B	463	HIS	N-CA-C	-5.45	101.28	109.95
1	A	373	ARG	O-C-N	-5.44	117.55	123.26
1	A	275	ARG	CD-NE-CZ	5.42	131.99	124.40
1	B	410	VAL	O-C-N	5.42	127.12	121.87
1	A	294	PRO	CA-C-N	-5.41	113.61	122.54
1	A	294	PRO	C-N-CA	-5.41	113.61	122.54
1	B	364	ASP	N-CA-C	5.41	122.32	110.80
1	B	327	MET	N-CA-C	-5.41	105.55	111.82
1	A	364	ASP	CA-CB-CG	-5.40	107.20	112.60
1	A	182	GLU	N-CA-C	5.39	117.26	108.63
1	B	325	ALA	CA-C-O	5.39	126.67	120.90
1	B	357	SER	N-CA-C	-5.38	106.67	113.18
1	A	278	PHE	N-CA-C	-5.36	104.01	110.44
1	B	402	VAL	CA-CB-CG2	5.36	119.50	110.40
1	B	379	GLY	CA-C-N	5.35	124.81	119.24
1	B	379	GLY	C-N-CA	5.35	124.81	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	382	CYS	N-CA-C	-5.35	105.53	111.36
1	B	391	PRO	N-CA-C	5.34	120.56	113.40
1	B	332	SER	CA-CB-OG	-5.34	100.42	111.10
1	A	441	ARG	CA-C-N	-5.32	114.48	122.47
1	A	441	ARG	C-N-CA	-5.32	114.48	122.47
1	B	441	ARG	CA-CB-CG	5.31	124.72	114.10
1	A	291	LEU	CB-CG-CD2	-5.31	94.78	110.70
1	B	484	VAL	CG1-CB-CG2	-5.30	99.14	110.80
1	A	267	ILE	O-C-N	-5.30	117.62	123.18
1	B	196	GLN	CB-CG-CD	-5.29	103.61	112.60
1	B	357	SER	O-C-N	-5.29	114.71	122.43
1	A	227	VAL	CG1-CB-CG2	-5.27	99.20	110.80
1	B	317	GLY	N-CA-C	-5.26	106.27	112.64
1	A	227	VAL	O-C-N	-5.26	116.97	122.81
1	B	477	THR	CA-C-N	5.26	129.87	122.09
1	B	477	THR	C-N-CA	5.26	129.87	122.09
1	B	244	HIS	CB-CA-C	-5.25	103.82	112.06
1	B	357	SER	CB-CA-C	5.25	120.39	109.95
1	B	357	SER	CA-C-N	-5.24	114.58	122.81
1	B	357	SER	C-N-CA	-5.24	114.58	122.81
1	B	464	LEU	CB-CA-C	-5.24	98.55	110.07
1	B	222	LYS	N-CA-C	5.24	119.42	113.19
1	A	488	ALA	CA-C-N	-5.23	113.91	122.54
1	A	488	ALA	C-N-CA	-5.23	113.91	122.54
1	B	367	ARG	CB-CA-C	5.23	119.16	110.90
1	A	363	LEU	N-CA-C	-5.23	105.02	111.40
1	A	446	PHE	CA-C-N	-5.20	114.90	122.86
1	A	446	PHE	C-N-CA	-5.20	114.90	122.86
1	B	379	GLY	N-CA-C	-5.20	101.74	112.34
1	B	375	PRO	CB-CG-CD	-5.19	89.50	106.10
1	B	473	PHE	CA-C-N	-5.18	115.69	123.00
1	B	473	PHE	C-N-CA	-5.18	115.69	123.00
1	A	231	LEU	N-CA-C	-5.17	100.30	108.73
1	B	384	LEU	N-CA-C	-5.17	105.76	111.71
1	A	461	TYR	CE1-CZ-OH	-5.16	104.44	119.90
1	A	239	VAL	N-CA-C	-5.15	100.15	107.77
1	B	370	GLU	CB-CA-C	5.12	119.32	110.77
1	B	401	GLY	CA-C-N	-5.11	115.82	122.51
1	B	401	GLY	C-N-CA	-5.11	115.82	122.51
1	A	410	VAL	CB-CA-C	-5.10	105.35	111.88
1	A	389	PRO	CA-C-O	-5.09	115.46	121.67
1	B	390	GLN	CA-C-N	5.09	124.40	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	390	GLN	C-N-CA	5.09	124.40	118.85
1	A	316	GLU	CB-CA-C	-5.09	101.39	110.70
1	A	472	GLN	CA-C-O	-5.08	114.89	120.43
1	A	301	ARG	CA-C-N	-5.08	114.41	121.67
1	A	301	ARG	C-N-CA	-5.08	114.41	121.67
1	A	425	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	B	412	LYS	N-CA-CB	-5.07	102.39	109.94
1	A	429	VAL	CA-C-O	-5.07	116.50	122.13
1	B	486	PRO	CB-CA-C	-5.07	104.92	111.46
1	B	472	GLN	CA-C-N	-5.05	115.75	122.72
1	B	472	GLN	C-N-CA	-5.05	115.75	122.72
1	A	385	LEU	CA-C-O	5.04	125.56	119.31
1	A	188	ILE	O-C-N	-5.03	116.28	122.57
1	A	298	HIS	N-CA-C	5.03	117.10	108.90
1	A	308	ASN	N-CA-CB	-5.03	102.69	110.13
1	A	302	GLY	O-C-N	-5.02	116.38	122.71
1	B	384	LEU	CA-C-N	-5.02	112.82	121.66
1	B	384	LEU	C-N-CA	-5.02	112.82	121.66
1	B	314	GLY	CA-C-N	-5.01	113.06	120.28
1	B	314	GLY	C-N-CA	-5.01	113.06	120.28
1	B	266	TYR	CB-CA-C	-5.00	99.96	109.66

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	LEU	Peptide
1	A	454	GLN	Peptide
1	B	465	GLN	Peptide
1	B	477	THR	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	2528	0	2462	131	0
1	B	2528	0	2462	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	34	0	0	12	1
3	B	22	0	0	6	0
All	All	5116	0	4924	246	1

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 25.

All (246) 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:A:399:LYS:CD	1:A:399:LYS:CE	1.77	1.60
1:B:194:LEU:CD2	1:B:194:LEU:CG	1.79	1.59
1:A:330:LEU:CD1	1:A:330:LEU:CG	1.79	1.58
1:A:206:ARG:CD	1:A:206:ARG:CG	1.75	1.58
1:B:479:VAL:CB	1:B:479:VAL:CG1	1.79	1.56
1:B:358:GLU:CD	1:B:358:GLU:CG	1.80	1.55
1:B:180:LYS:NZ	1:B:180:LYS:CE	1.68	1.54
1:A:233:GLU:CD	1:A:233:GLU:CG	1.80	1.52
1:A:358:GLU:CD	1:A:358:GLU:CG	1.81	1.50
1:A:399:LYS:CE	1:A:399:LYS:NZ	1.73	1.50
1:B:375:PRO:CG	1:B:375:PRO:CB	1.75	1.49
1:B:176:TYR:CD2	1:B:180:LYS:HE3	1.86	1.11
1:B:176:TYR:HD2	1:B:180:LYS:HE3	1.30	0.94
1:A:434:TYR:HE1	1:A:475:GLN:HE21	1.14	0.92
1:A:205:HIS:HD2	1:A:207:LYS:H	1.19	0.90
1:A:434:TYR:HE1	1:A:475:GLN:NE2	1.69	0.89
1:A:307:ASP:O	1:A:311:GLN:HG2	1.73	0.88
1:B:194:LEU:CD2	1:B:194:LEU:CB	2.54	0.85
1:B:307:ASP:O	1:B:311:GLN:HG2	1.76	0.84
1:A:206:ARG:CG	1:A:206:ARG:NE	2.41	0.83
1:A:298:HIS:HE1	3:A:33:HOH:O	1.62	0.83
1:A:176:TYR:CD2	1:A:180:LYS:HE3	2.14	0.83
1:A:233:GLU:HB2	3:A:13:HOH:O	1.78	0.82
1:B:242:ASP:HB3	1:B:244:HIS:CD2	2.14	0.82
1:B:176:TYR:CD2	1:B:180:LYS:CE	2.63	0.82
1:B:176:TYR:CE2	1:B:180:LYS:HE3	2.15	0.81
1:B:176:TYR:CE2	1:B:180:LYS:CE	2.63	0.80
1:B:479:VAL:CG1	1:B:479:VAL:CG2	2.60	0.78
1:B:217:LYS:HB2	1:B:334:VAL:HG22	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:TYR:HA	1:A:444:THR:O	1.85	0.76
1:B:412:LYS:NZ	1:B:416:GLU:OE2	2.19	0.76
1:A:176:TYR:CE2	1:A:180:LYS:CE	2.71	0.74
1:A:211:GLN:HG2	3:A:20:HOH:O	1.88	0.72
1:B:279:SER:HB2	1:B:318:GLU:OE1	1.90	0.72
1:A:176:TYR:CE2	1:A:180:LYS:HE3	2.26	0.71
1:B:292:LEU:O	1:B:292:LEU:HG	1.89	0.71
1:A:205:HIS:CD2	1:A:207:LYS:H	2.08	0.70
1:B:176:TYR:CE2	1:B:180:LYS:HE2	2.25	0.70
1:A:362:THR:HA	1:A:418:ASN:OD1	1.91	0.69
1:A:388:ASP:O	1:A:405:GLN:HA	1.92	0.69
1:B:307:ASP:HB3	1:B:311:GLN:HE21	1.56	0.69
1:A:246:GLN:HE22	1:A:451:TYR:HA	1.56	0.69
1:B:343:CYS:SG	1:B:346:GLY:HA2	2.33	0.69
1:B:182:GLU:O	1:B:183:ASP:HB2	1.93	0.68
1:A:206:ARG:CD	1:A:206:ARG:CB	2.69	0.68
1:B:271:ASP:OD1	1:B:304:HIS:HB2	1.94	0.67
1:A:335:PHE:O	1:A:337:TRP:N	2.28	0.66
1:A:425:ARG:HD3	1:A:425:ARG:C	2.21	0.66
1:B:329:GLU:O	1:B:333:GLU:HG3	1.96	0.65
1:A:307:ASP:HB3	1:A:311:GLN:HE21	1.61	0.65
1:A:330:LEU:CD1	1:A:330:LEU:HG	2.17	0.65
1:A:414:PHE:O	1:A:418:ASN:ND2	2.27	0.65
1:A:182:GLU:O	1:A:183:ASP:HB2	1.97	0.64
1:A:468:ASP:OD1	1:A:470:ARG:HB2	1.98	0.64
1:B:194:LEU:CD2	1:B:194:LEU:CD1	2.66	0.64
1:B:479:VAL:CG1	1:B:479:VAL:CA	2.71	0.63
1:A:176:TYR:CE2	1:A:180:LYS:HE2	2.34	0.63
1:A:176:TYR:CD2	1:A:180:LYS:CE	2.81	0.62
1:B:176:TYR:HE2	1:B:180:LYS:HE2	1.61	0.62
1:A:487:MET:O	1:A:489:TYR:N	2.33	0.62
1:A:351:MET:O	1:A:425:ARG:HA	2.00	0.62
1:A:281:GLU:OE1	1:A:281:GLU:N	2.25	0.61
1:B:432:GLU:HB3	1:B:475:GLN:NE2	2.16	0.61
1:B:307:ASP:HB3	1:B:311:GLN:NE2	2.16	0.60
1:A:204:LEU:HD11	1:A:208:CYS:CB	2.32	0.60
1:A:232:LYS:HD2	1:A:235:GLU:OE2	2.02	0.60
1:B:246:GLN:NE2	1:B:448:ALA:HB1	2.17	0.59
1:B:177:SER:HB3	3:B:36:HOH:O	2.02	0.59
1:A:345:ASN:HD22	1:A:469:LEU:HD21	1.68	0.59
1:B:176:TYR:HD2	1:B:180:LYS:CE	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:SER:HB2	1:A:474:HIS:O	2.03	0.59
1:A:317:GLY:HA3	1:A:489:TYR:O	2.04	0.58
1:B:205:HIS:HD2	1:B:207:LYS:H	1.51	0.58
1:B:474:HIS:CE1	3:B:19:HOH:O	2.54	0.58
1:A:176:TYR:HD2	1:A:180:LYS:HE3	1.68	0.58
1:A:412:LYS:NZ	1:A:416:GLU:OE2	2.36	0.58
1:B:212:ILE:O	1:B:213:LEU:C	2.43	0.58
1:B:432:GLU:HB3	1:B:475:GLN:HE21	1.69	0.58
1:A:305:GLU:CD	1:A:305:GLU:N	2.62	0.57
1:B:483:ASN:HB2	3:B:27:HOH:O	2.05	0.57
1:B:246:GLN:HE22	1:B:451:TYR:HA	1.70	0.57
1:B:452:CYS:O	1:B:453:ASP:HB2	2.04	0.57
1:A:274:ASP:O	1:A:275:ARG:HB2	2.05	0.56
1:A:487:MET:O	1:A:488:ALA:C	2.50	0.55
1:A:335:PHE:C	1:A:337:TRP:H	2.15	0.55
1:A:421:ASP:O	1:A:422:TYR:HB3	2.07	0.55
1:B:215:GLN:O	1:B:219:VAL:HG23	2.06	0.54
1:B:298:HIS:HD2	3:B:14:HOH:O	1.88	0.54
1:B:262:GLU:HG2	3:B:28:HOH:O	2.05	0.54
1:B:334:VAL:O	1:B:335:PHE:C	2.49	0.54
1:B:388:ASP:O	1:B:405:GLN:HA	2.06	0.54
1:A:241:GLY:O	1:A:242:ASP:C	2.48	0.54
1:A:205:HIS:HD2	1:A:207:LYS:N	1.99	0.54
1:A:335:PHE:C	1:A:337:TRP:N	2.63	0.54
1:B:445:VAL:HB	1:B:462:ILE:HD11	1.88	0.54
1:A:330:LEU:CD1	1:A:330:LEU:CB	2.78	0.54
1:B:232:LYS:HD2	1:B:235:GLU:OE2	2.08	0.54
1:A:434:TYR:CE1	1:A:475:GLN:NE2	2.62	0.53
1:A:364:ASP:OD2	1:A:368:LYS:NZ	2.39	0.53
1:A:246:GLN:NE2	3:A:6:HOH:O	2.41	0.53
1:B:242:ASP:HB3	1:B:244:HIS:HD2	1.67	0.53
1:A:330:LEU:CD1	1:A:330:LEU:CD2	2.77	0.53
1:B:319:VAL:O	1:B:323:TYR:N	2.29	0.53
1:A:248:TYR:CE1	1:A:482:PRO:HD2	2.45	0.52
1:B:392:GLN:OE1	1:B:392:GLN:N	2.27	0.52
1:A:305:GLU:CD	1:A:305:GLU:H	2.16	0.52
1:A:233:GLU:CD	1:A:233:GLU:CB	2.79	0.52
1:B:425:ARG:O	1:B:444:THR:HA	2.08	0.52
1:B:467:SER:O	1:B:468:ASP:HB2	2.09	0.52
1:B:485:LYS:O	1:B:488:ALA:HB2	2.09	0.52
1:A:436:VAL:HG22	1:A:443:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:TRP:CE2	1:B:202:LYS:HB3	2.45	0.52
1:B:176:TYR:HE2	1:B:180:LYS:CE	2.15	0.52
1:A:467:SER:O	1:A:468:ASP:CB	2.52	0.51
1:B:449:PRO:O	1:B:450:ASN:C	2.52	0.51
1:A:329:GLU:O	1:A:330:LEU:C	2.51	0.51
1:B:350:ILE:HA	1:B:424:ILE:O	2.10	0.51
1:A:236:LYS:HA	1:A:465:GLN:HA	1.93	0.51
1:B:429:VAL:HG11	1:B:455:MET:HE3	1.93	0.51
1:A:343:CYS:SG	1:A:346:GLY:HA2	2.51	0.50
1:B:310:ASN:HB2	1:B:328:TYR:OH	2.12	0.50
1:A:181:LEU:HB3	1:A:185:LYS:H	1.77	0.50
1:B:177:SER:CB	3:B:36:HOH:O	2.59	0.49
1:B:260:PRO:O	1:B:261:SER:HB3	2.12	0.49
1:B:360:GLY:HA2	1:B:417:GLU:OE2	2.11	0.49
1:B:242:ASP:OD1	1:B:242:ASP:N	2.46	0.49
1:A:350:ILE:HA	1:A:424:ILE:O	2.12	0.49
1:A:400:ARG:NH1	1:A:427:HIS:CE1	2.81	0.49
1:B:373:ARG:HG3	1:B:381:MET:HE1	1.95	0.49
1:A:216:VAL:O	1:A:217:LYS:C	2.56	0.49
1:B:205:HIS:CD2	1:B:207:LYS:H	2.31	0.48
1:A:411:THR:OG1	1:A:438:HIS:ND1	2.46	0.48
1:A:282:VAL:HG12	1:A:286:LEU:HD12	1.96	0.48
1:A:371:ARG:HH11	1:A:371:ARG:HG2	1.79	0.48
1:B:194:LEU:O	1:B:195:MET:C	2.55	0.48
1:B:232:LYS:H	1:B:235:GLU:HB2	1.78	0.48
1:B:282:VAL:HG12	1:B:286:LEU:HD12	1.95	0.48
1:A:229:THR:HG22	1:A:230:THR:N	2.29	0.48
1:A:225:THR:HG21	1:A:369:ILE:HB	1.96	0.48
1:B:467:SER:O	1:B:468:ASP:CB	2.62	0.48
1:A:467:SER:HB3	3:A:13:HOH:O	2.14	0.47
1:A:185:LYS:HE2	1:A:187:THR:HG22	1.95	0.47
1:B:194:LEU:CD2	1:B:194:LEU:HB3	2.44	0.47
1:A:345:ASN:ND2	1:A:469:LEU:HD21	2.29	0.47
1:B:210:TYR:HB2	1:B:327:MET:HE1	1.96	0.47
1:A:217:LYS:O	1:A:221:SER:HB3	2.14	0.47
1:B:243:THR:O	1:B:244:HIS:C	2.58	0.47
1:A:307:ASP:O	1:A:311:GLN:CG	2.55	0.47
1:A:334:VAL:O	1:A:335:PHE:C	2.57	0.47
1:A:325:ALA:O	1:A:329:GLU:HG2	2.15	0.47
1:A:373:ARG:NH1	3:A:44:HOH:O	2.46	0.47
1:A:449:PRO:O	1:A:450:ASN:C	2.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:SER:O	1:A:468:ASP:HB2	2.14	0.47
1:B:225:THR:CG2	1:B:340:LEU:HD12	2.44	0.47
1:B:362:THR:O	1:B:366:ILE:HG13	2.15	0.47
1:A:208:CYS:O	1:A:209:ALA:C	2.57	0.47
1:A:308:ASN:HB3	1:A:309:MET:HE2	1.96	0.47
1:A:314:GLY:O	1:A:315:PHE:C	2.55	0.46
1:A:335:PHE:O	1:A:338:LEU:HB2	2.15	0.46
1:B:335:PHE:O	1:B:337:TRP:N	2.47	0.46
1:B:252:ASN:O	1:B:253:ILE:C	2.56	0.46
1:B:347:LYS:HD3	1:B:347:LYS:HA	1.66	0.46
1:A:190:PHE:O	1:A:194:LEU:N	2.44	0.46
1:A:231:LEU:HD12	1:A:231:LEU:HA	1.47	0.46
1:B:309:MET:O	1:B:310:ASN:C	2.57	0.46
1:B:273:VAL:O	1:B:274:ASP:HB2	2.15	0.46
1:A:270:GLY:O	1:A:271:ASP:HB2	2.16	0.45
1:A:231:LEU:HB3	1:A:466:GLY:HA2	1.98	0.45
1:A:403:SER:N	3:A:56:HOH:O	2.22	0.45
1:B:279:SER:HB3	1:B:315:PHE:CD1	2.51	0.45
1:B:292:LEU:O	1:B:292:LEU:CG	2.59	0.45
1:A:394:GLY:H	1:A:409:ASP:CG	2.24	0.45
1:B:445:VAL:HB	1:B:462:ILE:CD1	2.46	0.45
1:A:429:VAL:HG12	3:A:23:HOH:O	2.17	0.45
1:B:314:GLY:O	1:B:318:GLU:N	2.48	0.45
1:A:398:SER:C	1:A:400:ARG:N	2.75	0.44
1:B:181:LEU:HD12	1:B:211:GLN:OE1	2.16	0.44
1:A:330:LEU:O	1:A:331:PHE:C	2.61	0.44
1:B:451:TYR:HB3	1:B:455:MET:HG3	1.98	0.44
1:A:358:GLU:HG3	3:A:1:HOH:O	2.16	0.44
1:A:460:SER:CB	1:A:474:HIS:O	2.66	0.44
1:B:314:GLY:O	1:B:315:PHE:C	2.58	0.44
1:A:215:GLN:O	1:A:218:GLU:HB3	2.18	0.44
1:B:186:VAL:HG12	1:B:187:THR:N	2.31	0.44
1:B:248:TYR:CD1	1:B:248:TYR:N	2.85	0.44
1:B:448:ALA:HA	1:B:449:PRO:HD2	1.86	0.44
1:B:351:MET:O	1:B:425:ARG:HA	2.17	0.44
1:A:393:ASN:HA	1:A:408:PRO:HD2	2.00	0.44
1:A:204:LEU:HD11	1:A:208:CYS:HB2	2.00	0.43
1:B:241:GLY:N	1:B:447:SER:OG	2.51	0.43
1:B:363:LEU:O	1:B:364:ASP:C	2.59	0.43
1:B:415:LEU:HD21	1:B:423:ILE:HG23	1.99	0.43
1:B:486:PRO:C	1:B:488:ALA:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:C	1:A:210:TYR:CD2	2.96	0.43
1:A:217:LYS:HE3	1:A:333:GLU:HB3	2.01	0.43
1:B:408:PRO:O	1:B:412:LYS:HB2	2.18	0.43
1:A:422:TYR:OH	1:A:471:PRO:HD3	2.18	0.43
1:B:402:VAL:O	1:B:403:SER:HB3	2.18	0.43
1:A:325:ALA:O	1:A:326:GLN:C	2.62	0.43
1:B:411:THR:OG1	1:B:438:HIS:ND1	2.50	0.43
1:A:452:CYS:O	1:A:454:GLN:HG3	2.19	0.43
1:B:232:LYS:HD2	1:B:235:GLU:CD	2.43	0.43
1:A:329:GLU:O	1:A:333:GLU:HG3	2.18	0.43
1:A:335:PHE:O	1:A:336:GLU:C	2.61	0.43
1:B:206:ARG:O	1:B:209:ALA:HB3	2.19	0.42
1:B:383:ASP:O	1:B:384:LEU:C	2.59	0.42
1:A:437:ALA:HB2	3:A:25:HOH:O	2.18	0.42
1:A:392:GLN:O	1:A:392:GLN:HG2	2.19	0.42
1:B:274:ASP:CG	1:B:313:TYR:HB2	2.44	0.42
1:B:335:PHE:C	1:B:337:TRP:N	2.77	0.42
1:A:310:ASN:N	1:A:310:ASN:HD22	2.16	0.42
1:B:336:GLU:O	1:B:372:ASN:HA	2.20	0.42
1:B:451:TYR:O	1:B:452:CYS:HB2	2.18	0.42
1:A:237:ILE:HG21	1:A:237:ILE:HD13	1.83	0.42
1:A:188:ILE:HD13	1:A:188:ILE:O	2.19	0.42
1:A:428:GLU:HA	3:A:23:HOH:O	2.19	0.42
1:B:198:TYR:HD1	1:B:198:TYR:HA	1.58	0.42
1:B:429:VAL:CG2	1:B:430:LYS:N	2.83	0.42
1:A:211:GLN:O	1:A:215:GLN:HG3	2.19	0.42
1:B:364:ASP:OD2	1:B:368:LYS:NZ	2.47	0.42
1:B:382:CYS:O	1:B:383:ASP:C	2.62	0.41
1:A:246:GLN:HG2	3:A:6:HOH:O	2.19	0.41
1:A:479:VAL:HB	1:A:480:PRO:CD	2.50	0.41
1:A:292:LEU:O	1:A:292:LEU:HG	2.21	0.41
1:A:302:GLY:N	1:A:305:GLU:OE1	2.52	0.41
1:A:336:GLU:O	1:A:372:ASN:HA	2.21	0.41
1:B:194:LEU:HA	1:B:194:LEU:HD12	1.89	0.41
1:A:290:LYS:HA	1:A:290:LYS:HD3	1.91	0.41
1:B:325:ALA:O	1:B:326:GLN:C	2.62	0.41
1:A:273:VAL:O	1:A:274:ASP:HB2	2.21	0.41
1:A:415:LEU:HD21	1:A:423:ILE:HG23	2.01	0.41
1:B:198:TYR:CD1	1:B:281:GLU:HG3	2.56	0.41
1:A:243:THR:O	1:A:246:GLN:HG3	2.21	0.41
1:B:352:HIS:O	1:B:427:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:TYR:CZ	1:A:205:HIS:HB2	2.56	0.41
1:A:212:ILE:O	1:A:213:LEU:C	2.64	0.41
1:A:274:ASP:CG	1:A:313:TYR:HB2	2.46	0.41
1:B:406:PHE:HB2	1:B:410:VAL:HG11	2.03	0.41
1:B:231:LEU:HD12	1:B:231:LEU:HA	1.53	0.40
1:A:487:MET:C	1:A:489:TYR:N	2.79	0.40
1:B:241:GLY:O	1:B:242:ASP:C	2.64	0.40
1:A:206:ARG:H	1:A:206:ARG:HG2	1.77	0.40
1:A:275:ARG:NH1	1:A:451:TYR:OH	2.55	0.40
1:A:355:LEU:HA	1:A:355:LEU:HD23	1.84	0.40
1:A:445:VAL:HB	1:A:462:ILE:HD11	2.03	0.40
1:B:213:LEU:HD12	1:B:327:MET:SD	2.61	0.40

All (1) 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)
3:A:1:HOH:O	3:A:30:HOH:O[4_445]	2.09	0.11

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	313/315 (99%)	274 (88%)	33 (10%)	6 (2%)	6 13
1	B	313/315 (99%)	276 (88%)	27 (9%)	10 (3%)	3 5
All	All	626/630 (99%)	550 (88%)	60 (10%)	16 (3%)	4 7

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	ASP

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Mol	Chain	Res	Type
1	B	393	ASN
1	B	450	ASN
1	B	468	ASP
1	A	377	ASP
1	B	372	ASN
1	A	320	LYS
1	B	233	GLU
1	B	261	SER
1	B	427	HIS
1	B	488	ALA
1	A	217	LYS
1	A	274	ASP
1	A	393	ASN
1	A	488	ALA
1	B	364	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	279/279 (100%)	248 (89%)	31 (11%)	5 10
1	B	279/279 (100%)	241 (86%)	38 (14%)	3 5
All	All	558/558 (100%)	489 (88%)	69 (12%)	4 7

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	188	ILE
1	A	211	GLN
1	A	214	VAL
1	A	222	LYS
1	A	231	LEU
1	A	232	LYS
1	A	233	GLU

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Mol	Chain	Res	Type
1	A	235	GLU
1	A	242	ASP
1	A	246	GLN
1	A	267	ILE
1	A	280	VAL
1	A	329	GLU
1	A	358	GLU
1	A	366	ILE
1	A	368	LYS
1	A	398	SER
1	A	399	LYS
1	A	400	ARG
1	A	402	VAL
1	A	409	ASP
1	A	419	ASN
1	A	424	ILE
1	A	425	ARG
1	A	447	SER
1	A	455	MET
1	A	465	GLN
1	A	468	ASP
1	A	486	PRO
1	A	487	MET
1	B	180	LYS
1	B	183	ASP
1	B	185	LYS
1	B	188	ILE
1	B	198	TYR
1	B	200	ASP
1	B	203	LYS
1	B	204	LEU
1	B	211	GLN
1	B	214	VAL
1	B	216	VAL
1	B	231	LEU
1	B	234	THR
1	B	235	GLU
1	B	242	ASP
1	B	243	THR
1	B	280	VAL
1	B	326	GLN
1	B	344	ILE

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Mol	Chain	Res	Type
1	B	347	LYS
1	B	364	ASP
1	B	366	ILE
1	B	370	GLU
1	B	373	ARG
1	B	377	ASP
1	B	397	ILE
1	B	398	SER
1	B	399	LYS
1	B	402	VAL
1	B	419	ASN
1	B	423	ILE
1	B	425	ARG
1	B	441	ARG
1	B	455	MET
1	B	465	GLN
1	B	470	ARG
1	B	472	GLN
1	B	487	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	246	GLN
1	A	264	ASN
1	A	296	HIS
1	A	298	HIS
1	A	310	ASN
1	A	311	GLN
1	A	454	GLN
1	A	472	GLN
1	A	474	HIS
1	B	205	HIS
1	B	246	GLN
1	B	264	ASN
1	B	298	HIS
1	B	310	ASN
1	B	311	GLN
1	B	419	ASN
1	B	454	GLN
1	B	472	GLN

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Mol	Chain	Res	Type
1	B	475	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	315/315 (100%)	-0.50	0	100	100	1, 2, 5, 17	4 (1%)
1	B	315/315 (100%)	-0.41	0	100	100	1, 2, 11, 24	4 (1%)
All	All	630/630 (100%)	-0.45	0	100	100	1, 2, 8, 24	8 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	B	501	1/1	0.98	0.03	25,25,25,25	0
2	ZN	A	501	1/1	0.99	0.03	8,8,8,8	0
2	ZN	B	500	1/1	0.99	0.02	2,2,2,2	0
2	ZN	A	500	1/1	0.99	0.02	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.