Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:05 AM GMT

PDB ID	:	3H66
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

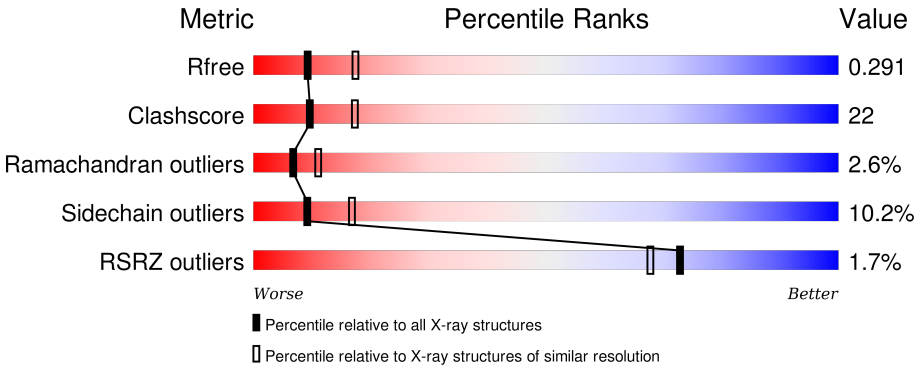
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.59 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	% 32% 45% 17% 5%
1	B	315	2% 36% 44% 17% .

2 Entry composition

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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is water.

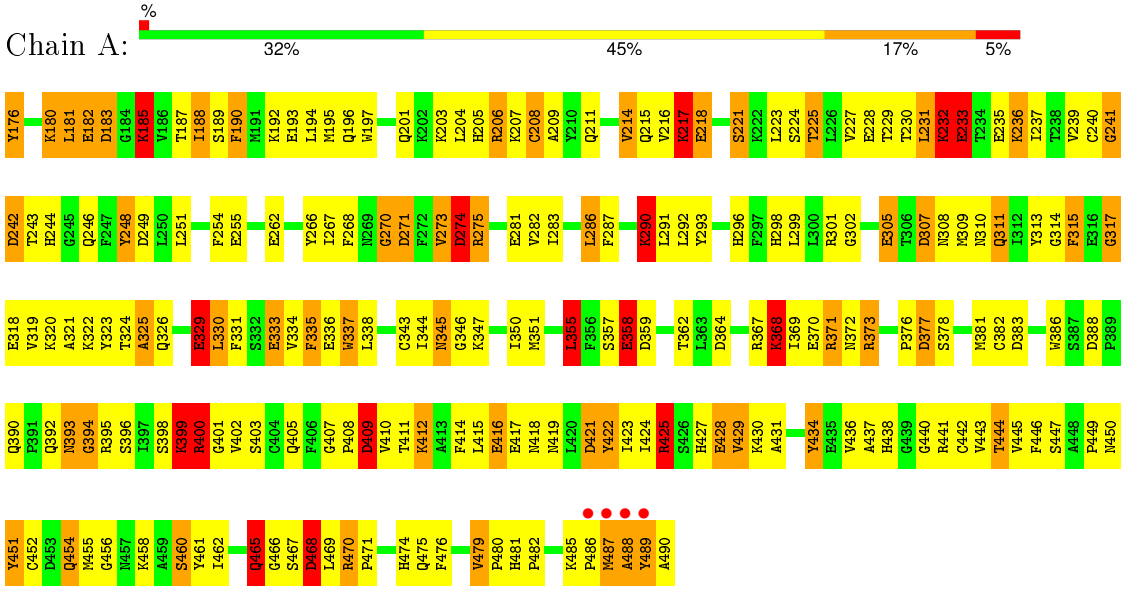
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	22	Total	O	0	0
			22	22		

3 Residue-property plots (i)

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

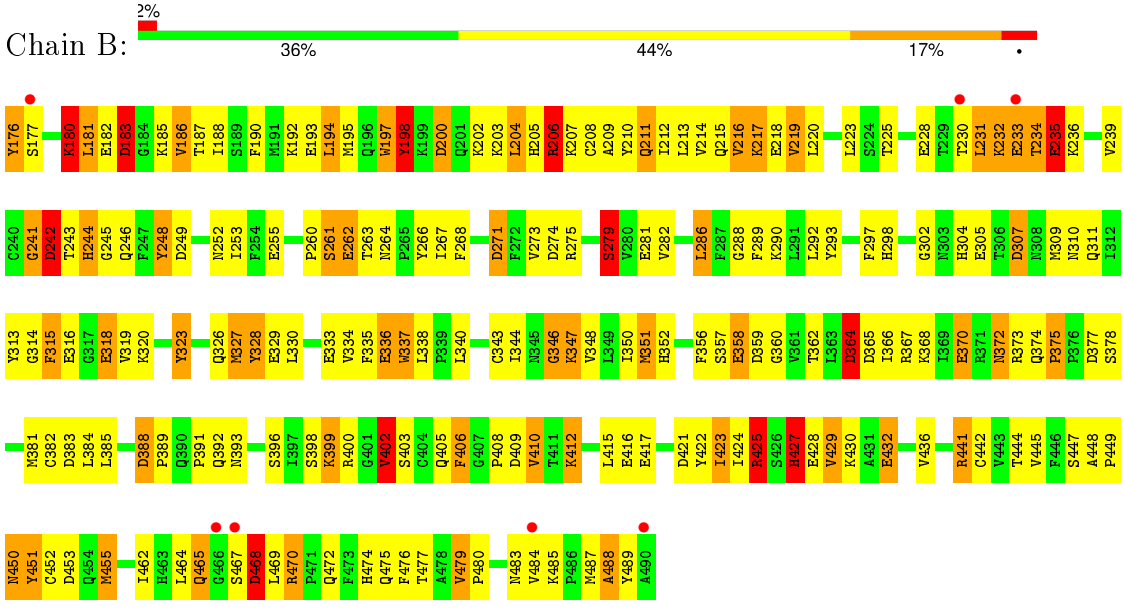
- Molecule 1: Serine/threonine-protein phosphatase 5

Chain A:



- Molecule 1: Serine/threonine-protein phosphatase 5

Chain B:



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) 92.2 (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 (10.16%)	DCC
Wilson B-factor (Å^2)	4.4	Xtriage
Anisotropy	1.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 32.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 19742 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	2.58	151/2592 (5.8%)	1.96	67/3506 (1.9%)
1	B	2.46	130/2592 (5.0%)	1.88	67/3506 (1.9%)
All	All	2.52	281/5184 (5.4%)	1.92	134/7012 (1.9%)

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 (281) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	GLU	CG-CD	19.66	1.81	1.51
1	A	233	GLU	CG-CD	19.14	1.80	1.51
1	B	358	GLU	CG-CD	18.69	1.79	1.51
1	A	417	GLU	CB-CG	-14.13	1.25	1.52
1	B	255	GLU	CD-OE1	13.13	1.40	1.25
1	B	479	VAL	CB-CG1	12.68	1.79	1.52
1	A	255	GLU	CB-CG	-12.44	1.28	1.52
1	A	370	GLU	CG-CD	12.07	1.70	1.51
1	B	358	GLU	CD-OE1	11.28	1.38	1.25
1	A	417	GLU	CG-CD	-11.25	1.35	1.51
1	A	370	GLU	CD-OE2	11.19	1.38	1.25
1	A	262	GLU	CD-OE1	10.90	1.37	1.25
1	B	208	CYS	CB-SG	-10.61	1.64	1.82
1	B	422	TYR	CD1-CE1	10.59	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	LYS	CD-CE	10.42	1.77	1.51
1	B	218	GLU	CD-OE2	10.04	1.36	1.25
1	B	216	VAL	CB-CG1	-9.98	1.31	1.52
1	B	218	GLU	CG-CD	9.98	1.67	1.51
1	B	315	PHE	CE2-CZ	9.88	1.56	1.37
1	A	268	PHE	CE1-CZ	-9.87	1.18	1.37
1	A	399	LYS	CE-NZ	9.72	1.73	1.49
1	B	358	GLU	CD-OE2	9.68	1.36	1.25
1	B	198	TYR	CE1-CZ	9.54	1.50	1.38
1	B	198	TYR	CD2-CE2	-9.51	1.25	1.39
1	A	254	PHE	CE2-CZ	9.45	1.55	1.37
1	B	442	CYS	CB-SG	9.39	1.98	1.82
1	A	293	TYR	CD2-CE2	-9.38	1.25	1.39
1	A	206	ARG	CG-CD	9.27	1.75	1.51
1	B	428	GLU	CD-OE1	9.23	1.35	1.25
1	A	323	TYR	CE2-CZ	-9.19	1.26	1.38
1	B	218	GLU	CD-OE1	8.94	1.35	1.25
1	A	214	VAL	CA-CB	8.73	1.73	1.54
1	B	216	VAL	C-O	8.67	1.39	1.23
1	A	358	GLU	CD-OE2	8.57	1.35	1.25
1	A	180	LYS	CD-CE	8.49	1.72	1.51
1	A	434	TYR	CE1-CZ	8.44	1.49	1.38
1	B	370	GLU	C-O	8.39	1.39	1.23
1	A	266	TYR	CB-CG	-8.37	1.39	1.51
1	B	479	VAL	CB-CG2	-8.36	1.35	1.52
1	B	297	PHE	CG-CD1	8.28	1.51	1.38
1	A	381	MET	C-O	-8.16	1.07	1.23
1	A	233	GLU	CD-OE2	8.10	1.34	1.25
1	A	244	HIS	N-CA	8.03	1.62	1.46
1	A	182	GLU	CG-CD	8.01	1.64	1.51
1	B	194	LEU	C-O	8.01	1.38	1.23
1	B	176	TYR	CE1-CZ	7.98	1.49	1.38
1	A	470	ARG	CZ-NH1	7.91	1.43	1.33
1	B	484	VAL	CB-CG2	-7.81	1.36	1.52
1	B	180	LYS	CE-NZ	7.81	1.68	1.49
1	A	315	PHE	CG-CD1	7.71	1.50	1.38
1	B	210	TYR	CD1-CE1	7.70	1.50	1.39
1	B	217	LYS	CD-CE	7.68	1.70	1.51
1	A	479	VAL	CB-CG2	7.68	1.69	1.52
1	A	239	VAL	CB-CG1	-7.67	1.36	1.52
1	B	316	GLU	CB-CG	7.65	1.66	1.52
1	A	305	GLU	CG-CD	7.58	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	268	PHE	CD2-CE2	-7.57	1.24	1.39
1	A	358	GLU	CD-OE1	7.52	1.33	1.25
1	B	197	TRP	CG-CD1	7.42	1.47	1.36
1	A	401	GLY	N-CA	7.40	1.57	1.46
1	B	328	TYR	CE2-CZ	7.36	1.48	1.38
1	A	330	LEU	CG-CD1	7.36	1.79	1.51
1	B	305	GLU	CD-OE2	7.35	1.33	1.25
1	B	194	LEU	CG-CD2	7.34	1.79	1.51
1	B	275	ARG	CZ-NH1	7.34	1.42	1.33
1	A	185	LYS	CD-CE	7.32	1.69	1.51
1	B	429	VAL	C-O	-7.32	1.09	1.23
1	A	193	GLU	CB-CG	-7.32	1.38	1.52
1	A	429	VAL	C-O	-7.21	1.09	1.23
1	B	470	ARG	CB-CG	7.21	1.72	1.52
1	B	228	GLU	CB-CG	-7.20	1.38	1.52
1	B	422	TYR	CE2-CZ	-7.20	1.29	1.38
1	A	395	ARG	CZ-NH2	-7.13	1.23	1.33
1	B	198	TYR	CG-CD2	7.12	1.48	1.39
1	B	382	CYS	CB-SG	-7.12	1.70	1.82
1	A	325	ALA	C-O	7.12	1.36	1.23
1	B	315	PHE	CG-CD1	7.12	1.49	1.38
1	A	248	TYR	CD2-CE2	7.09	1.50	1.39
1	B	370	GLU	CD-OE1	7.09	1.33	1.25
1	B	262	GLU	CD-OE1	7.06	1.33	1.25
1	A	431	ALA	CA-CB	-7.05	1.37	1.52
1	A	180	LYS	CE-NZ	7.05	1.66	1.49
1	A	382	CYS	CB-SG	-7.01	1.70	1.82
1	B	356	PHE	CE1-CZ	6.96	1.50	1.37
1	A	326	GLN	CD-OE1	6.95	1.39	1.24
1	A	275	ARG	NE-CZ	6.94	1.42	1.33
1	A	176	TYR	CB-CG	6.94	1.62	1.51
1	A	373	ARG	C-O	-6.94	1.10	1.23
1	A	248	TYR	CD1-CE1	6.93	1.49	1.39
1	A	407	GLY	C-O	-6.90	1.12	1.23
1	B	412	LYS	CD-CE	6.90	1.68	1.51
1	B	410	VAL	C-O	6.89	1.36	1.23
1	A	262	GLU	CG-CD	6.87	1.62	1.51
1	B	468	ASP	CB-CG	6.84	1.66	1.51
1	A	315	PHE	CE2-CZ	6.83	1.50	1.37
1	B	356	PHE	CE2-CZ	6.82	1.50	1.37
1	A	331	PHE	CE2-CZ	-6.82	1.24	1.37
1	B	356	PHE	CD2-CE2	6.81	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	489	TYR	CG-CD1	6.81	1.48	1.39
1	A	456	GLY	N-CA	-6.80	1.35	1.46
1	A	422	TYR	CG-CD2	6.77	1.48	1.39
1	A	197	TRP	CG-CD1	6.77	1.46	1.36
1	A	446	PHE	CD1-CE1	6.75	1.52	1.39
1	B	328	TYR	CG-CD2	6.72	1.47	1.39
1	B	451	TYR	CB-CG	6.70	1.61	1.51
1	A	370	GLU	CD-OE1	6.68	1.33	1.25
1	A	390	GLN	C-O	-6.67	1.10	1.23
1	A	176	TYR	CG-CD2	6.64	1.47	1.39
1	A	251	LEU	C-O	-6.64	1.10	1.23
1	B	268	PHE	CD2-CE2	6.61	1.52	1.39
1	A	470	ARG	CZ-NH2	6.61	1.41	1.33
1	A	311	GLN	CG-CD	6.58	1.66	1.51
1	B	297	PHE	CE2-CZ	6.56	1.49	1.37
1	A	347	LYS	CD-CE	6.54	1.67	1.51
1	B	266	TYR	CZ-OH	6.52	1.49	1.37
1	A	206	ARG	C-O	-6.51	1.10	1.23
1	A	358	GLU	CB-CG	6.49	1.64	1.52
1	B	297	PHE	CD1-CE1	6.49	1.52	1.39
1	A	262	GLU	CD-OE2	6.47	1.32	1.25
1	A	217	LYS	CE-NZ	6.43	1.65	1.49
1	B	441	ARG	CZ-NH1	6.38	1.41	1.33
1	B	241	GLY	N-CA	6.34	1.55	1.46
1	A	410	VAL	N-CA	6.33	1.59	1.46
1	B	219	VAL	CB-CG1	6.32	1.66	1.52
1	B	320	LYS	CE-NZ	6.31	1.64	1.49
1	A	441	ARG	NE-CZ	6.31	1.41	1.33
1	B	436	VAL	CB-CG1	6.30	1.66	1.52
1	A	347	LYS	C-O	-6.28	1.11	1.23
1	A	218	GLU	CD-OE2	6.28	1.32	1.25
1	B	422	TYR	CD2-CE2	6.27	1.48	1.39
1	A	434	TYR	CB-CG	-6.23	1.42	1.51
1	A	233	GLU	CD-OE1	6.20	1.32	1.25
1	B	176	TYR	CD2-CE2	6.20	1.48	1.39
1	A	227	VAL	CB-CG1	-6.20	1.39	1.52
1	B	289	PHE	CE1-CZ	6.19	1.49	1.37
1	B	315	PHE	CE1-CZ	6.18	1.49	1.37
1	B	348	VAL	CB-CG2	-6.18	1.39	1.52
1	B	180	LYS	C-O	6.16	1.35	1.23
1	B	476	PHE	CE1-CZ	6.16	1.49	1.37
1	B	192	LYS	CE-NZ	6.15	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	PHE	CG-CD1	6.14	1.48	1.38
1	B	406	PHE	CB-CG	-6.14	1.41	1.51
1	A	296	HIS	CA-C	6.13	1.69	1.52
1	A	267	ILE	N-CA	-6.12	1.34	1.46
1	B	428	GLU	CD-OE2	6.12	1.32	1.25
1	A	224	SER	C-O	-6.12	1.11	1.23
1	A	451	TYR	CE2-CZ	-6.12	1.30	1.38
1	A	193	GLU	CG-CD	-6.11	1.42	1.51
1	A	490	ALA	CA-CB	6.11	1.65	1.52
1	B	211	GLN	CG-CD	6.10	1.65	1.51
1	A	318	GLU	CB-CG	6.07	1.63	1.52
1	A	481	HIS	C-O	6.04	1.34	1.23
1	A	196	GLN	CB-CG	6.03	1.68	1.52
1	A	377	ASP	N-CA	6.00	1.58	1.46
1	B	186	VAL	CB-CG1	5.99	1.65	1.52
1	A	197	TRP	CB-CG	5.97	1.60	1.50
1	A	485	LYS	CB-CG	5.95	1.68	1.52
1	A	322	LYS	CE-NZ	-5.95	1.34	1.49
1	A	460	SER	C-O	5.94	1.34	1.23
1	B	228	GLU	CD-OE2	5.93	1.32	1.25
1	B	279	SER	C-O	5.90	1.34	1.23
1	A	321	ALA	CA-CB	5.89	1.64	1.52
1	B	206	ARG	CZ-NH1	5.87	1.40	1.33
1	B	399	LYS	CB-CG	5.87	1.68	1.52
1	A	430	LYS	C-O	-5.86	1.12	1.23
1	A	176	TYR	CE1-CZ	5.86	1.46	1.38
1	B	337	TRP	CG-CD1	5.86	1.45	1.36
1	A	228	GLU	CG-CD	-5.85	1.43	1.51
1	B	210	TYR	CE2-CZ	5.84	1.46	1.38
1	A	416	GLU	CG-CD	5.84	1.60	1.51
1	B	480	PRO	CG-CD	5.83	1.69	1.50
1	A	293	TYR	CD1-CE1	-5.83	1.30	1.39
1	A	270	GLY	C-O	-5.82	1.14	1.23
1	A	441	ARG	CD-NE	5.82	1.56	1.46
1	B	219	VAL	CA-CB	5.81	1.67	1.54
1	B	318	GLU	CG-CD	5.81	1.60	1.51
1	A	266	TYR	CD1-CE1	-5.81	1.30	1.39
1	A	333	GLU	CD-OE1	5.81	1.32	1.25
1	B	244	HIS	N-CA	5.80	1.57	1.46
1	A	221	SER	CB-OG	5.80	1.49	1.42
1	A	283	ILE	C-O	5.78	1.34	1.23
1	B	180	LYS	CD-CE	5.78	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	VAL	CB-CG1	5.77	1.65	1.52
1	A	476	PHE	CD2-CE2	5.77	1.50	1.39
1	A	176	TYR	CA-C	5.76	1.68	1.52
1	A	193	GLU	N-CA	-5.75	1.34	1.46
1	A	308	ASN	CB-CG	-5.75	1.37	1.51
1	B	194	LEU	CA-CB	-5.75	1.40	1.53
1	B	268	PHE	C-O	5.72	1.34	1.23
1	B	206	ARG	NE-CZ	5.71	1.40	1.33
1	B	245	GLY	N-CA	-5.71	1.37	1.46
1	A	345	ASN	CG-OD1	-5.70	1.11	1.24
1	A	331	PHE	CD1-CE1	-5.70	1.27	1.39
1	A	193	GLU	C-O	5.70	1.34	1.23
1	A	254	PHE	CG-CD2	5.69	1.47	1.38
1	B	396	SER	N-CA	5.67	1.57	1.46
1	B	436	VAL	CB-CG2	5.67	1.64	1.52
1	B	451	TYR	CE1-CZ	5.66	1.46	1.38
1	B	206	ARG	CG-CD	5.65	1.66	1.51
1	B	236	LYS	N-CA	5.65	1.57	1.46
1	A	444	THR	CB-CG2	-5.65	1.33	1.52
1	A	489	TYR	CG-CD2	5.63	1.46	1.39
1	B	406	PHE	CG-CD2	-5.63	1.30	1.38
1	B	183	ASP	CB-CG	5.62	1.63	1.51
1	A	268	PHE	CG-CD2	-5.62	1.30	1.38
1	A	428	GLU	CD-OE1	5.62	1.31	1.25
1	A	458	LYS	N-CA	-5.61	1.35	1.46
1	B	389	PRO	CA-C	5.61	1.64	1.52
1	A	376	PRO	C-O	5.59	1.34	1.23
1	A	275	ARG	CG-CD	5.58	1.66	1.51
1	A	287	PHE	CE1-CZ	-5.58	1.26	1.37
1	A	460	SER	CB-OG	5.56	1.49	1.42
1	B	239	VAL	CB-CG1	-5.56	1.41	1.52
1	B	338	LEU	C-O	-5.54	1.12	1.23
1	B	323	TYR	CG-CD1	5.54	1.46	1.39
1	B	293	TYR	CG-CD2	5.53	1.46	1.39
1	B	383	ASP	CB-CG	5.51	1.63	1.51
1	A	465	GLN	CD-NE2	5.50	1.46	1.32
1	B	441	ARG	NE-CZ	5.48	1.40	1.33
1	A	248	TYR	CZ-OH	5.46	1.47	1.37
1	B	235	GLU	CD-OE2	5.45	1.31	1.25
1	A	468	ASP	C-O	5.43	1.33	1.23
1	A	440	GLY	C-O	-5.43	1.15	1.23
1	A	185	LYS	CG-CD	5.42	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	189	SER	CB-OG	-5.42	1.35	1.42
1	B	391	PRO	C-O	5.39	1.34	1.23
1	B	271	ASP	CB-CG	5.39	1.63	1.51
1	B	263	THR	CB-CG2	5.38	1.70	1.52
1	A	208	CYS	C-O	5.38	1.33	1.23
1	B	365	ASP	CA-CB	-5.37	1.42	1.53
1	B	336	GLU	CB-CG	-5.36	1.42	1.52
1	A	236	LYS	CB-CG	5.34	1.67	1.52
1	B	370	GLU	CG-CD	5.34	1.59	1.51
1	A	425	ARG	CZ-NH1	5.34	1.40	1.33
1	B	234	THR	CA-CB	5.34	1.67	1.53
1	A	255	GLU	CA-CB	-5.34	1.42	1.53
1	A	273	VAL	N-CA	-5.34	1.35	1.46
1	B	315	PHE	CB-CG	-5.33	1.42	1.51
1	B	451	TYR	CE2-CZ	-5.33	1.31	1.38
1	B	399	LYS	CG-CD	5.32	1.70	1.52
1	B	248	TYR	CE2-CZ	-5.29	1.31	1.38
1	B	374	GLN	CA-C	5.29	1.66	1.52
1	B	288	GLY	C-O	5.29	1.32	1.23
1	B	302	GLY	C-O	5.28	1.32	1.23
1	A	326	GLN	CD-NE2	5.28	1.46	1.32
1	A	225	THR	N-CA	-5.26	1.35	1.46
1	A	319	VAL	CB-CG2	-5.25	1.41	1.52
1	B	356	PHE	CB-CG	-5.24	1.42	1.51
1	A	330	LEU	CA-C	5.23	1.66	1.52
1	B	290	LYS	CE-NZ	5.21	1.62	1.49
1	A	290	LYS	C-O	5.21	1.33	1.23
1	A	240	CYS	CB-SG	-5.20	1.73	1.81
1	B	313	TYR	CG-CD2	5.19	1.45	1.39
1	B	268	PHE	CE1-CZ	-5.19	1.27	1.37
1	A	489	TYR	N-CA	5.18	1.56	1.46
1	A	412	LYS	CE-NZ	5.18	1.61	1.49
1	A	412	LYS	CD-CE	5.16	1.64	1.51
1	A	476	PHE	CE1-CZ	-5.16	1.27	1.37
1	A	355	LEU	CG-CD2	-5.16	1.32	1.51
1	A	367	ARG	C-O	-5.15	1.13	1.23
1	B	289	PHE	CE2-CZ	5.14	1.47	1.37
1	B	375	PRO	CB-CG	5.14	1.75	1.50
1	A	337	TRP	CE3-CZ3	5.14	1.47	1.38
1	A	241	GLY	C-O	-5.13	1.15	1.23
1	B	206	ARG	N-CA	5.13	1.56	1.46
1	A	322	LYS	CG-CD	5.12	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	VAL	CB-CG1	5.11	1.63	1.52
1	B	255	GLU	CB-CG	-5.11	1.42	1.52
1	A	313	TYR	CD1-CE1	-5.11	1.31	1.39
1	A	395	ARG	C-O	-5.11	1.13	1.23
1	A	337	TRP	N-CA	5.11	1.56	1.46
1	B	373	ARG	CB-CG	5.11	1.66	1.52
1	B	190	PHE	CE2-CZ	5.09	1.47	1.37
1	B	268	PHE	CD1-CE1	5.08	1.49	1.39
1	A	201	GLN	C-O	-5.08	1.13	1.23
1	A	287	PHE	CD2-CE2	-5.08	1.29	1.39
1	B	248	TYR	CD1-CE1	5.04	1.47	1.39
1	A	370	GLU	C-O	5.04	1.32	1.23
1	A	335	PHE	C-O	5.03	1.32	1.23
1	B	264	ASN	CG-OD1	5.03	1.35	1.24
1	B	406	PHE	CE1-CZ	-5.01	1.27	1.37

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	367	ARG	NE-CZ-NH2	-15.80	112.40	120.30
1	A	367	ARG	NE-CZ-NH1	15.31	127.95	120.30
1	A	400	ARG	NE-CZ-NH1	-14.33	113.14	120.30
1	B	385	LEU	CB-CG-CD2	-12.80	89.24	111.00
1	B	384	LEU	CB-CG-CD2	-12.00	90.61	111.00
1	B	194	LEU	CB-CG-CD1	-11.38	91.66	111.00
1	B	359	ASP	CB-CG-OD2	-11.38	108.06	118.30
1	A	425	ARG	NE-CZ-NH2	-11.33	114.64	120.30
1	A	183	ASP	CB-CG-OD1	11.31	128.48	118.30
1	A	368	LYS	CD-CE-NZ	-11.03	86.34	111.70
1	B	400	ARG	NE-CZ-NH1	-10.72	114.94	120.30
1	A	275	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	B	409	ASP	CB-CG-OD1	10.20	127.48	118.30
1	B	236	LYS	CD-CE-NZ	-10.09	88.50	111.70
1	A	271	ASP	CB-CG-OD2	-10.07	109.24	118.30
1	A	425	ARG	NE-CZ-NH1	10.03	125.32	120.30
1	B	206	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	A	395	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	A	383	ASP	CB-CG-OD2	-9.58	109.68	118.30
1	A	291	LEU	CB-CG-CD2	-9.54	94.78	111.00
1	A	183	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	B	421	ASP	CB-CG-OD2	9.17	126.56	118.30
1	B	255	GLU	OE1-CD-OE2	9.00	134.10	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	400	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	B	378	SER	N-CA-CB	-8.61	97.58	110.50
1	A	274	ASP	CB-CG-OD1	-8.61	110.56	118.30
1	B	469	LEU	CB-CG-CD1	-8.53	96.50	111.00
1	B	470	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	A	249	ASP	CB-CG-OD2	8.14	125.63	118.30
1	A	180	LYS	CD-CE-NZ	8.14	130.41	111.70
1	A	299	LEU	CB-CG-CD1	-8.05	97.32	111.00
1	B	181	LEU	CB-CG-CD2	-7.95	97.48	111.00
1	A	355	LEU	CB-CG-CD2	-7.91	97.55	111.00
1	A	421	ASP	CB-CG-OD2	7.90	125.41	118.30
1	A	181	LEU	CB-CG-CD1	7.89	124.42	111.00
1	A	441	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	468	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	377	ASP	CB-CA-C	-7.70	95.00	110.40
1	B	409	ASP	CB-CG-OD2	-7.68	111.39	118.30
1	A	206	ARG	CG-CD-NE	-7.68	95.68	111.80
1	B	220	LEU	CB-CG-CD2	-7.64	98.01	111.00
1	A	203	LYS	CB-CG-CD	-7.55	91.96	111.60
1	A	301	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	A	421	ASP	CB-CG-OD1	-7.51	111.54	118.30
1	B	255	GLU	CG-CD-OE2	-7.46	103.39	118.30
1	B	441	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	B	271	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	484	VAL	CG1-CB-CG2	-7.35	99.14	110.90
1	B	307	ASP	CB-CG-OD1	-7.33	111.70	118.30
1	A	227	VAL	CG1-CB-CG2	-7.31	99.20	110.90
1	B	183	ASP	N-CA-C	-7.25	91.44	111.00
1	B	223	LEU	CB-CG-CD1	-7.22	98.73	111.00
1	B	388	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	A	358	GLU	N-CA-C	-6.99	92.13	111.00
1	B	388	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	249	ASP	CB-CG-OD1	-6.88	112.11	118.30
1	B	198	TYR	CG-CD1-CE1	-6.86	115.81	121.30
1	B	425	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	271	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	359	ASP	CB-CG-OD1	6.62	124.25	118.30
1	A	446	PHE	CB-CA-C	-6.61	97.17	110.40
1	A	223	LEU	CB-CG-CD1	-6.48	99.98	111.00
1	B	399	LYS	CD-CE-NZ	6.42	126.48	111.70
1	B	192	LYS	CD-CE-NZ	6.39	126.40	111.70
1	A	359	ASP	CB-CG-OD2	-6.39	112.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195	MET	CG-SD-CE	6.38	110.41	100.20
1	B	399	LYS	CB-CG-CD	6.31	128.01	111.60
1	B	464	LEU	CA-CB-CG	6.29	129.75	115.30
1	B	242	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	B	381	MET	CG-SD-CE	6.23	110.17	100.20
1	A	378	SER	N-CA-C	-6.23	94.18	111.00
1	B	427	HIS	N-CA-CB	-6.22	99.41	110.60
1	B	200	ASP	CB-CG-OD2	6.18	123.86	118.30
1	B	230	THR	CA-CB-CG2	-6.16	103.78	112.40
1	B	217	LYS	CD-CE-NZ	6.15	125.83	111.70
1	B	464	LEU	CB-CA-C	-6.13	98.55	110.20
1	A	383	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	357	SER	O-C-N	-6.13	112.90	122.70
1	B	233	GLU	CB-CA-C	6.13	122.65	110.40
1	B	327	MET	CG-SD-CE	6.07	109.90	100.20
1	A	236	LYS	CD-CE-NZ	-6.05	97.79	111.70
1	A	231	LEU	CA-CB-CG	-6.01	101.48	115.30
1	A	275	ARG	CD-NE-CZ	6.00	131.99	123.60
1	B	180	LYS	CD-CE-NZ	5.92	125.31	111.70
1	B	286	LEU	CB-CG-CD2	-5.91	100.95	111.00
1	A	344	ILE	CB-CA-C	-5.86	99.88	111.60
1	A	381	MET	CG-SD-CE	5.85	109.56	100.20
1	A	468	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	461	TYR	CE1-CZ-OH	-5.80	104.44	120.10
1	B	373	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	249	ASP	OD1-CG-OD2	-5.78	112.32	123.30
1	B	464	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	A	417	GLU	CB-CA-C	-5.74	98.92	110.40
1	B	402	VAL	CA-CB-CG2	5.74	119.50	110.90
1	A	192	LYS	C-N-CA	-5.72	107.40	121.70
1	A	371	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	275	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	203	LYS	CD-CE-NZ	-5.68	98.63	111.70
1	B	242	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	275	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	B	346	GLY	N-CA-C	-5.65	98.98	113.10
1	B	464	LEU	CB-CG-CD1	5.63	120.56	111.00
1	A	441	ARG	NH1-CZ-NH2	-5.58	113.27	119.40
1	B	206	ARG	NH1-CZ-NH2	-5.57	113.27	119.40
1	A	394	GLY	N-CA-C	5.56	127.01	113.10
1	B	344	ILE	CB-CA-C	-5.56	100.47	111.60
1	A	409	ASP	CB-CG-OD1	5.56	123.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	244	HIS	CB-CA-C	-5.56	99.29	110.40
1	B	193	GLU	N-CA-CB	5.53	120.56	110.60
1	B	236	LYS	CA-CB-CG	-5.53	101.23	113.40
1	A	232	LYS	CA-CB-CG	5.51	125.52	113.40
1	A	317	GLY	N-CA-C	-5.48	99.40	113.10
1	A	470	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	233	GLU	CA-CB-CG	5.47	125.44	113.40
1	B	330	LEU	CB-CG-CD1	5.47	120.30	111.00
1	A	329	GLU	C-N-CA	-5.46	108.06	121.70
1	B	357	SER	CB-CA-C	5.42	120.39	110.10
1	B	204	LEU	CB-CG-CD1	-5.40	101.83	111.00
1	B	432	GLU	CA-C-N	5.38	126.97	116.20
1	A	275	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
1	A	386	TRP	N-CA-C	5.26	125.22	111.00
1	A	309	MET	CG-SD-CE	-5.24	91.82	100.20
1	B	266	TYR	CB-CA-C	-5.22	99.96	110.40
1	B	367	ARG	N-CA-C	-5.16	97.06	111.00
1	A	461	TYR	CB-CG-CD2	5.16	124.09	121.00
1	A	396	SER	N-CA-CB	5.15	118.22	110.50
1	B	441	ARG	CA-CB-CG	5.15	124.72	113.40
1	A	307	ASP	CB-CG-OD1	-5.14	113.68	118.30
1	B	421	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	B	232	LYS	CD-CE-NZ	-5.08	100.01	111.70
1	A	396	SER	CA-CB-OG	5.07	124.89	111.20
1	B	267	ILE	CB-CA-C	-5.05	101.51	111.60
1	A	324	THR	CB-CA-C	-5.04	97.99	111.60
1	A	286	LEU	CA-CB-CG	-5.03	103.72	115.30

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	123	0
1	B	2528	0	2462	101	0
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	224	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 22.

All (224) 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:CE	1:A:399:LYS:CD	1.77	1.60
1:B:194:LEU:CG	1:B:194:LEU:CD2	1.79	1.59
1:A:330:LEU:CD1	1:A:330:LEU:CG	1.79	1.58
1:A:206:ARG:CG	1:A:206:ARG:CD	1.75	1.58
1:B:479:VAL:CG1	1:B:479:VAL:CB	1.79	1.56
1:B:180:LYS:CE	1:B:180:LYS:NZ	1.68	1.54
1:B:358:GLU:CD	1:B:358:GLU:CG	1.80	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:A:358:GLU:CD	1:A:358:GLU:CG	1.81	1.49
1:A:233:GLU:CG	1:A:233:GLU:CD	1.80	1.47
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:CB	1:B:194:LEU:CD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG2	1:B:479:VAL:CG1	2.60	0.78
1:B:217:LYS:HB2	1:B:334:VAL:HG22	1.64	0.78
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:CB	1:A:206:ARG:CD	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: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:HG	1:A:330:LEU:CD1	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:B:176:TYR:HE2	1:B:180:LYS:HE2	1.61	0.62
1:A:176:TYR:CD2	1:A:180:LYS:CE	2.81	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:425:ARG:HD3	1:A:425:ARG:C	2.21	0.61
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:232:LYS:HD2	1:A:235:GLU:OE2	2.02	0.60
1:A:204:LEU:HD11	1:A:208:CYS:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:176:TYR:HD2	1:B:180:LYS:CE	2.09	0.59
1:A:345:ASN:HD22	1:A:469:LEU:HD21	1.68	0.59
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:B:432:GLU:HB3	1:B:475:GLN:HE21	1.69	0.58
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:467:SER:O	1:A:468:ASP:CB	2.52	0.56
1:A:412:LYS:NZ	1:A:416:GLU:OE2	2.36	0.56
1:A:274:ASP:O	1:A:275:ARG:HB2	2.05	0.56
1:B:212:ILE:O	1:B:213:LEU:C	2.43	0.56
1:A:421:ASP:O	1:A:422:TYR:HB3	2.07	0.55
1:B:298:HIS:HD2	3:B:14:HOH:O	1.88	0.54
1:B:215:GLN:O	1:B:219:VAL:HG23	2.06	0.54
1:B:262:GLU:HG2	3:B:28:HOH:O	2.05	0.54
1:B:388:ASP:O	1:B:405:GLN:HA	2.06	0.54
1:A:205:HIS:HD2	1:A:207:LYS:N	1.99	0.54
1:B:445:VAL:HB	1:B:462:ILE:HD11	1.88	0.54
1:A:330:LEU:CB	1:A:330:LEU:CD1	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: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:305:GLU:N	1:A:305:GLU:CD	2.62	0.53
1:A:330:LEU:CD2	1:A:330:LEU:CD1	2.77	0.53
1:B:319:VAL:O	1:B:323:TYR:N	2.29	0.53
1:B:392:GLN:N	1:B:392:GLN:OE1	2.27	0.52
1:A:248:TYR:CE1	1:A:482:PRO:HD2	2.45	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
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:335:PHE:C	1:A:337:TRP:N	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:MET:O	1:A:488:ALA:C	2.50	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:310:ASN:HB2	1:B:328:TYR:OH	2.12	0.50
1:A:343:CYS:SG	1:A:346:GLY:HA2	2.51	0.50
1:A:181:LEU:HB3	1:A:185:LYS:H	1.77	0.50
1:A:335:PHE:C	1:A:337:TRP:H	2.15	0.50
1:B:334:VAL:O	1:B:335:PHE:C	2.49	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:A:241:GLY:O	1:A:242:ASP:C	2.48	0.49
1:B:242:ASP:N	1:B:242:ASP:OD1	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:205:HIS:CD2	1:B:207:LYS:H	2.31	0.48
1:A:411:THR:HG1	1:A:438:HIS:CE1	2.28	0.48
1:A:282:VAL:HG12	1:A:286:LEU:HD12	1.96	0.48
1:A:371:ARG:HG2	1:A:371:ARG:HH11	1.79	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:B:467:SER:O	1:B:468:ASP:CB	2.62	0.48
1:A:225:THR:HG21	1:A:369:ILE:HB	1.96	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:HB3	1:B:194:LEU:CD2	2.44	0.47
1:A:305:GLU:CD	1:A:305:GLU:H	2.16	0.47
1:A:345:ASN:ND2	1:A:469:LEU:HD21	2.29	0.47
1:A:217:LYS:O	1:A:221:SER:HB3	2.14	0.47
1:A:307:ASP:O	1:A:311:GLN:CG	2.55	0.47
1:A:325:ALA:O	1:A:329:GLU:HG2	2.15	0.47
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:A:373:ARG:NH1	3:A:44:HOH:O	2.46	0.47
1:A:364:ASP:OD2	1:A:368:LYS:NZ	2.39	0.47
1:B:362:THR:O	1:B:366:ILE:HG13	2.15	0.47
1:B:449:PRO:O	1:B:450:ASN:C	2.52	0.46
1:A:329:GLU:O	1:A:330:LEU:C	2.51	0.46
1:B:335:PHE:O	1:B:337:TRP:N	2.47	0.46
1:A:335:PHE:O	1:A:338:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:VAL:O	1:B:274:ASP:HB2	2.15	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:HA	1:A:231:LEU:HD12	1.47	0.46
1:A:270:GLY:O	1:A:271:ASP:HB2	2.16	0.45
1:B:279:SER:HB3	1:B:315:PHE:CD1	2.51	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:292:LEU:O	1:B:292:LEU:CG	2.59	0.45
1:B:445:VAL:HB	1:B:462:ILE:CD1	2.46	0.45
1:B:314:GLY:O	1:B:318:GLU:N	2.48	0.45
1:A:429:VAL:HG12	3:A:23:HOH:O	2.17	0.45
1:A:314:GLY:O	1:A:315:PHE:C	2.55	0.45
1:B:181:LEU:HD12	1:B:211:GLN:OE1	2.16	0.44
1:B:451:TYR:HB3	1:B:455:MET:HG3	1.98	0.44
1:A:216:VAL:O	1:A:217:LYS:C	2.56	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:A:215:GLN:O	1:A:218:GLU:HB3	2.18	0.44
1:B:194:LEU:O	1:B:195:MET:C	2.55	0.44
1:B:448:ALA:HA	1:B:449:PRO:HD2	1.86	0.44
1:B:248:TYR:CD1	1:B:248:TYR:N	2.85	0.44
1:B:186:VAL:HG12	1:B:187:THR:N	2.31	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:233:GLU:CB	1:A:233:GLU:CD	2.79	0.43
1:A:204:LEU:HD11	1:A:208:CYS:HB2	2.00	0.43
1:B:415:LEU:HD21	1:B:423:ILE:HG23	1.99	0.43
1:B:241:GLY:N	1:B:447:SER:OG	2.51	0.43
1:A:487:MET:HE3	1:A:487:MET:HB2	1.94	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:452:CYS:O	1:A:454:GLN:HG3	2.19	0.43
1:A:329:GLU:O	1:A:333:GLU:HG3	2.18	0.43
1:B:206:ARG:O	1:B:209:ALA:HB3	2.19	0.42
1:B:243:THR:O	1:B:244:HIS:C	2.58	0.42
1:A:437:ALA:HB2	3:A:25:HOH:O	2.18	0.42
1:A:334:VAL:O	1:A:335:PHE:C	2.57	0.42
1:A:392:GLN:O	1:A:392:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASN:N	1:A:310:ASN:HD22	2.16	0.42
1:A:449:PRO:O	1:A:450:ASN:C	2.56	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:208:CYS:O	1:A:209:ALA:C	2.57	0.42
1:A:237:ILE:HD13	1:A:237:ILE:HG21	1.83	0.42
1:A:428:GLU:HA	3:A:23:HOH:O	2.19	0.42
1:A:188:ILE:O	1:A:188:ILE:HD13	2.19	0.42
1:B:429:VAL:CG2	1:B:430:LYS:N	2.83	0.42
1:B:198:TYR:HD1	1:B:198:TYR:HA	1.58	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: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:B:194:LEU:HD12	1:B:194:LEU:HA	1.89	0.41
1:A:302:GLY:N	1:A:305:GLU:OE1	2.52	0.41
1:A:292:LEU:O	1:A:292:LEU:HG	2.21	0.41
1:B:252:ASN:O	1:B:253:ILE:C	2.56	0.41
1:A:336:GLU:O	1:A:372:ASN:HA	2.21	0.41
1:A:290:LYS:HD3	1:A:290:LYS:HA	1.91	0.41
1:A:273:VAL:O	1:A:274:ASP:HB2	2.21	0.41
1:B:309:MET:O	1:B:310:ASN:C	2.57	0.41
1:B:198:TYR:CD1	1:B:281:GLU:HG3	2.56	0.41
1:A:415:LEU:HD21	1:A:423:ILE:HG23	2.01	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
1:A:176:TYR:CZ	1:A:205:HIS:HB2	2.56	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:206:ARG:HG2	1:A:206:ARG:H	1.77	0.40
1:A:275:ARG:NH1	1:A:451:TYR:OH	2.55	0.40
1:B:213:LEU:HD12	1:B:327:MET:SD	2.61	0.40
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.84	0.40
1:A:445:VAL:HB	1:A:462:ILE:HD11	2.03	0.40
1:A:394:GLY:H	1:A:409:ASP:CG	2.24	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%)	10 19
1	B	313/315 (99%)	276 (88%)	27 (9%)	10 (3%)	5 8
All	All	626/630 (99%)	550 (88%)	60 (10%)	16 (3%)	7 11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	ASP
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%)	255 (91%)	24 (9%)	13 25
1	B	279/279 (100%)	246 (88%)	33 (12%)	6 12
All	All	558/558 (100%)	501 (90%)	57 (10%)	9 17

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	LYS
1	A	188	ILE
1	A	214	VAL
1	A	232	LYS
1	A	233	GLU
1	A	242	ASP
1	A	290	LYS
1	A	329	GLU
1	A	358	GLU
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	425	ARG
1	A	442	CYS
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	206	ARG
1	B	214	VAL
1	B	216	VAL

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Mol	Chain	Res	Type
1	B	231	LEU
1	B	234	THR
1	B	235	GLU
1	B	242	ASP
1	B	279	SER
1	B	326	GLN
1	B	347	LYS
1	B	351	MET
1	B	364	ASP
1	B	370	GLU
1	B	377	ASP
1	B	398	SER
1	B	399	LYS
1	B	402	VAL
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	246	GLN
1	A	264	ASN
1	A	298	HIS
1	A	310	ASN
1	A	311	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	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 carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	315/315 (100%)	-0.17	4 (1%)	79	75	2, 2, 5, 17	4 (1%)
1	B	315/315 (100%)	-0.04	7 (2%)	65	59	2, 2, 11, 24	4 (1%)
All	All	630/630 (100%)	-0.10	11 (1%)	73	68	2, 2, 8, 24	8 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	467	SER	3.4
1	B	230	THR	3.1
1	B	466	GLY	3.0
1	A	487	MET	2.7
1	A	489	TYR	2.7
1	B	177	SER	2.6
1	A	488	ALA	2.5
1	A	486	PRO	2.2
1	B	233	GLU	2.2
1	B	490	ALA	2.1
1	B	484	VAL	2.1

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	ZN	A	500	1/1	0.99	0.03	-6.17	2,2,2,2	0
2	ZN	B	501	1/1	0.98	0.04	-6.29	25,25,25,25	0
2	ZN	A	501	1/1	0.99	0.03	-6.87	8,8,8,8	0
2	ZN	B	500	1/1	0.99	0.03	-8.77	2,2,2,2	0

6.5 Other polymers (i)

There are no such residues in this entry.