



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:15 AM UTC

PDB ID : 2WDP / pdb_00002wdp
Title : Crystal Structure of Ligand Free Human Caspase-6
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Deposited on : 2009-03-25
Resolution : 1.95 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

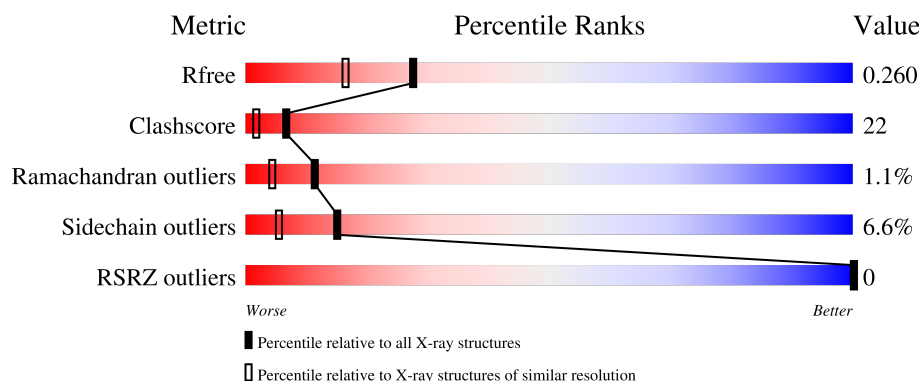
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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 $\leq 5\%$. 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	293	
1	B	293	
1	C	293	
1	D	293	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7539 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 CASPASE-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1806	1155	317	321	13			
1	B	227	Total	C	N	O	S	0	0	0
			1833	1172	320	328	13			
1	C	227	Total	C	N	O	S	0	0	0
			1833	1170	321	328	14			
1	D	230	Total	C	N	O	S	0	0	0
			1855	1185	324	332	14			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

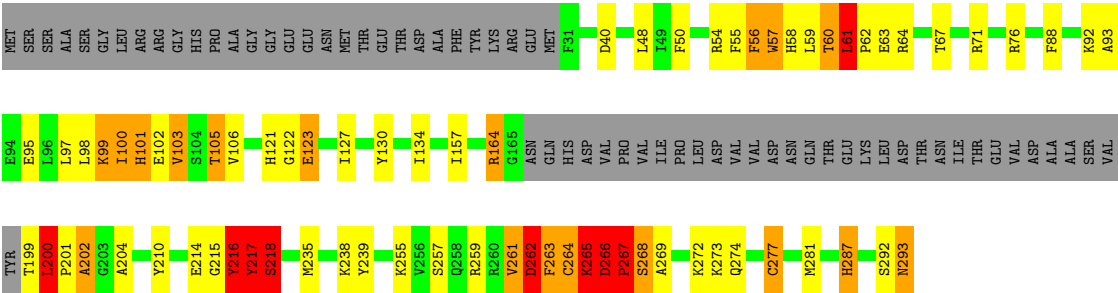


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total 58	O 58	0	0
3	B	45	Total 45	O 45	0	0
3	C	47	Total 47	O 47	0	0
3	D	57	Total 57	O 57	0	0

● Molecule 1: CASPASE-6



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.15Å 90.44Å 86.40Å 90.00° 92.77° 90.00°	Depositor
Resolution (Å)	63.07 – 1.95 63.07 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (63.07-1.95) 97.7 (63.07-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.224 , 0.262 0.228 , 0.260	Depositor DCC
R_{free} test set	3458 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7539	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.07	3/1848 (0.2%)	2.12	54/2481 (2.2%)
1	B	1.05	4/1876 (0.2%)	1.47	25/2521 (1.0%)
1	C	1.01	3/1876 (0.2%)	1.42	22/2519 (0.9%)
1	D	1.05	3/1899 (0.2%)	1.94	44/2552 (1.7%)
All	All	1.05	13/7499 (0.2%)	1.76	145/10073 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	8
1	B	0	1
1	C	1	2
1	D	1	6
All	All	3	17

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	LYS	CA-C	-9.94	1.42	1.52
1	C	256	VAL	CA-CB	-6.71	1.46	1.54
1	C	270	ILE	CA-CB	6.38	1.61	1.54
1	A	92	LYS	N-CA	-6.05	1.39	1.46
1	B	159	ILE	CA-CB	-5.57	1.47	1.54
1	B	48	LEU	C-O	-5.55	1.17	1.24
1	C	273	LYS	N-CA	-5.46	1.39	1.46
1	D	287	HIS	CE1-NE2	-5.16	1.27	1.32
1	D	157	ILE	C-O	-5.15	1.18	1.24
1	D	277	CYS	CB-SG	-5.11	1.64	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	127	ILE	CA-CB	-5.10	1.48	1.54
1	A	93	ALA	CA-C	5.04	1.59	1.52
1	B	282	LEU	CA-C	-5.00	1.46	1.52

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	SER	N-CA-C	28.66	155.41	111.56
1	A	213	ALA	N-CA-C	26.18	166.56	110.80
1	D	265	LYS	N-CA-CB	-25.46	69.52	110.51
1	C	57	TRP	N-CA-C	-24.95	75.65	108.34
1	B	93	ALA	CB-CA-C	-22.36	83.49	111.22
1	D	123	GLU	N-CA-C	22.24	141.73	111.92
1	A	202	ALA	CA-C-N	22.17	140.44	121.82
1	A	202	ALA	C-N-CA	22.17	140.44	121.82
1	D	218	SER	CA-C-N	22.07	163.68	121.54
1	D	218	SER	C-N-CA	22.07	163.68	121.54
1	B	292	SER	N-CA-C	22.05	143.10	112.45
1	A	213	ALA	CA-C-N	19.76	159.28	121.54
1	A	213	ALA	C-N-CA	19.76	159.28	121.54
1	D	262	ASP	CB-CA-C	-19.24	72.14	110.42
1	D	262	ASP	N-CA-C	18.73	150.69	110.80
1	A	214	GLU	N-CA-C	18.37	149.94	110.80
1	D	268	SER	N-CA-CB	-18.07	82.63	110.46
1	A	272	LYS	N-CA-C	17.39	147.84	110.80
1	A	269	ALA	N-CA-C	16.64	133.39	112.92
1	A	268	SER	CA-C-N	14.50	145.85	122.65
1	A	268	SER	C-N-CA	14.50	145.85	122.65
1	A	268	SER	CB-CA-C	-14.09	84.68	111.03
1	D	92	LYS	N-CA-C	-14.01	86.40	109.24
1	A	273	LYS	CB-CA-C	13.74	137.77	110.42
1	D	123	GLU	CA-C-N	13.66	137.85	120.64
1	D	123	GLU	C-N-CA	13.66	137.85	120.64
1	A	57	TRP	CB-CA-C	13.39	137.05	111.48
1	A	213	ALA	CB-CA-C	-13.25	84.05	110.42
1	D	92	LYS	CB-CA-C	13.15	131.45	109.75
1	D	262	ASP	CA-C-N	12.43	141.85	122.08
1	D	262	ASP	C-N-CA	12.43	141.85	122.08
1	A	214	GLU	CB-CA-C	-12.34	85.86	110.42
1	D	268	SER	N-CA-C	-11.99	98.88	113.15
1	D	266	ASP	C-N-CD	-11.92	94.38	120.60
1	A	273	LYS	CA-C-N	11.91	139.78	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	LYS	C-N-CA	11.91	139.78	122.99
1	D	264	CYS	N-CA-C	11.84	131.89	113.19
1	B	216	TYR	N-CA-C	11.80	128.50	109.85
1	D	266	ASP	N-CA-C	11.52	135.26	109.81
1	A	42	ARG	NE-CZ-NH2	11.32	129.39	119.20
1	B	57	TRP	CB-CA-C	-11.26	88.02	110.42
1	C	65	ARG	NE-CZ-NH2	11.14	129.22	119.20
1	C	65	ARG	NE-CZ-NH1	-10.92	110.58	121.50
1	D	265	LYS	N-CA-C	10.91	126.65	110.17
1	D	215	GLY	N-CA-C	10.86	138.92	113.18
1	C	273	LYS	CA-C-N	10.75	142.07	121.54
1	C	273	LYS	C-N-CA	10.75	142.07	121.54
1	A	214	GLU	CA-C-N	10.75	142.47	121.41
1	A	214	GLU	C-N-CA	10.75	142.47	121.41
1	D	265	LYS	CB-CA-C	-10.73	90.14	111.60
1	D	164	ARG	NE-CZ-NH2	10.54	128.69	119.20
1	A	42	ARG	NE-CZ-NH1	-10.54	110.96	121.50
1	A	267	PRO	CB-CA-C	10.21	129.50	110.10
1	A	212	VAL	CB-CA-C	10.14	126.45	110.52
1	B	92	LYS	N-CA-C	-10.14	92.00	108.52
1	D	122	GLY	O-C-N	10.08	131.64	122.77
1	B	292	SER	CB-CA-C	-10.07	91.07	110.11
1	D	61	LEU	N-CA-C	9.83	131.54	109.81
1	D	164	ARG	NE-CZ-NH1	-9.79	111.71	121.50
1	A	122	GLY	N-CA-C	9.76	136.30	113.18
1	C	292	SER	N-CA-C	9.62	125.25	109.95
1	D	218	SER	N-CA-C	9.46	130.94	110.80
1	D	93	ALA	N-CA-C	9.35	122.47	111.71
1	A	57	TRP	CA-C-N	9.34	135.32	122.34
1	A	57	TRP	C-N-CA	9.34	135.32	122.34
1	C	274	GLN	N-CA-C	-9.23	91.14	110.80
1	C	56	PHE	CB-CA-C	-9.15	90.26	109.38
1	A	92	LYS	N-CA-C	-9.12	101.05	112.72
1	B	92	LYS	CB-CA-C	8.72	124.50	110.19
1	C	65	ARG	CD-NE-CZ	8.71	136.59	124.40
1	A	57	TRP	N-CA-C	-8.71	97.41	109.95
1	A	42	ARG	CD-NE-CZ	8.70	136.57	124.40
1	A	216	TYR	N-CA-C	8.18	128.22	110.80
1	A	71	ARG	NE-CZ-NH2	8.13	126.52	119.20
1	A	267	PRO	N-CA-C	-8.11	91.82	112.10
1	A	215	GLY	N-CA-C	8.04	132.22	113.18
1	D	123	GLU	CB-CA-C	-8.04	100.70	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	273	LYS	N-CA-C	7.99	127.81	110.80
1	A	71	ARG	NE-CZ-NH1	-7.51	113.99	121.50
1	A	202	ALA	CB-CA-C	-7.46	95.50	113.19
1	D	259	ARG	NE-CZ-NH2	7.43	125.89	119.20
1	C	71	ARG	NE-CZ-NH2	7.34	125.80	119.20
1	D	164	ARG	CD-NE-CZ	7.32	134.65	124.40
1	D	216	TYR	CA-C-N	7.25	133.86	120.95
1	D	216	TYR	C-N-CA	7.25	133.86	120.95
1	D	61	LEU	CB-CA-C	-7.24	95.91	110.17
1	D	217	TYR	N-CA-CB	-7.22	100.47	110.29
1	A	201	PRO	N-CA-C	-7.13	97.79	112.47
1	C	57	TRP	CB-CA-C	7.05	129.91	113.19
1	D	200	LEU	N-CA-CB	-7.02	97.87	110.37
1	D	259	ARG	NE-CZ-NH1	-6.99	114.52	121.50
1	A	202	ALA	N-CA-C	-6.97	99.20	108.34
1	A	200	LEU	CA-C-N	6.92	128.49	119.84
1	A	200	LEU	C-N-CA	6.92	128.49	119.84
1	B	259	ARG	NE-CZ-NH2	6.88	125.39	119.20
1	A	270	ILE	CB-CA-C	-6.72	100.26	111.29
1	B	216	TYR	CA-C-N	6.64	130.55	121.05
1	B	216	TYR	C-N-CA	6.64	130.55	121.05
1	B	32	ASP	CA-C-N	6.62	126.31	119.56
1	B	32	ASP	C-N-CA	6.62	126.31	119.56
1	B	259	ARG	NE-CZ-NH1	-6.54	114.97	121.50
1	C	71	ARG	NE-CZ-NH1	-6.46	115.03	121.50
1	A	215	GLY	CA-C-N	6.35	133.68	121.54
1	A	215	GLY	C-N-CA	6.35	133.68	121.54
1	A	259	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	C	245	PHE	N-CA-C	6.25	118.09	111.28
1	A	271	GLY	N-CA-C	6.22	127.93	113.18
1	B	215	GLY	N-CA-C	-6.16	104.88	112.77
1	D	71	ARG	NE-CZ-NH2	-6.12	113.70	119.20
1	A	272	LYS	N-CA-CB	-6.06	100.24	110.49
1	A	259	ARG	CD-NE-CZ	6.06	132.88	124.40
1	C	71	ARG	CD-NE-CZ	6.00	132.80	124.40
1	B	277	CYS	N-CA-C	-5.90	99.73	108.99
1	D	92	LYS	CA-C-N	5.83	128.68	120.28
1	D	92	LYS	C-N-CA	5.83	128.68	120.28
1	A	96	LEU	N-CA-C	-5.78	104.35	111.40
1	C	56	PHE	N-CA-C	-5.77	100.39	109.50
1	A	239	TYR	N-CA-C	5.74	120.99	113.30
1	B	71	ARG	NE-CZ-NH2	-5.71	114.06	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	ASP	CA-C-N	5.70	126.96	119.84
1	A	32	ASP	C-N-CA	5.70	126.96	119.84
1	B	71	ARG	CD-NE-CZ	5.67	132.34	124.40
1	C	260	ARG	N-CA-C	-5.62	105.16	111.28
1	B	202	ALA	N-CA-C	5.59	115.22	107.73
1	B	58	HIS	CA-C-N	-5.58	113.33	122.26
1	B	58	HIS	C-N-CA	-5.58	113.33	122.26
1	D	71	ARG	CD-NE-CZ	5.56	132.18	124.40
1	D	216	TYR	O-C-N	5.50	128.94	121.74
1	D	56	PHE	N-CA-C	-5.44	101.67	110.32
1	C	60	THR	N-CA-C	-5.41	103.56	110.53
1	D	71	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	B	281	MET	N-CA-C	-5.39	104.27	111.87
1	A	71	ARG	CD-NE-CZ	5.36	131.90	124.40
1	C	274	GLN	N-CA-CB	5.36	119.54	110.49
1	C	93	ALA	N-CA-C	5.35	122.19	110.80
1	A	281	MET	CA-CB-CG	-5.31	103.48	114.10
1	D	202	ALA	N-CA-C	5.26	116.41	108.46
1	B	200	LEU	C-N-CD	-5.22	103.61	125.00
1	D	101	HIS	N-CA-C	-5.22	106.87	113.18
1	A	272	LYS	CB-CA-C	-5.20	100.07	110.42
1	C	101	HIS	CA-C-N	5.18	128.18	120.31
1	C	101	HIS	C-N-CA	5.18	128.18	120.31
1	B	216	TYR	CA-C-O	5.13	127.46	121.46
1	B	57	TRP	N-CA-C	5.04	121.55	110.80
1	B	73	ASN	N-CA-C	-5.04	105.67	111.07

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	213	ALA	CA
1	C	273	LYS	CA
1	D	218	SER	CA

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	202	ALA	Peptide
1	A	213	ALA	Peptide
1	A	214	GLU	Peptide
1	A	215	GLY	Peptide
1	A	268	SER	Peptide

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Mol	Chain	Res	Type	Group
1	A	273	LYS	Peptide
1	A	92	LYS	Peptide
1	A	93	ALA	Peptide
1	B	215	GLY	Peptide
1	C	216	TYR	Peptide
1	C	292	SER	Peptide
1	D	217	TYR	Peptide
1	D	218	SER	Peptide
1	D	262	ASP	Peptide
1	D	265	LYS	Peptide
1	D	266	ASP	Peptide
1	D	267	PRO	Peptide

5.2 Too-close contacts

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	1806	0	1787	68	3
1	B	1833	0	1807	86	4
1	C	1833	0	1805	68	4
1	D	1855	0	1829	105	4
2	D	5	0	0	0	0
3	A	58	0	0	5	0
3	B	45	0	0	4	0
3	C	47	0	0	0	0
3	D	57	0	0	4	0
All	All	7539	0	7228	313	8

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LYS:CA	1:D:265:LYS:HE2	1.49	1.33
1:A:93:ALA:HB1	1:A:96:LEU:N	1.59	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:LYS:HE2	1:D:265:LYS:HA	1.16	1.14
1:D:265:LYS:CA	1:D:265:LYS:CE	2.29	1.11
1:A:217:TYR:HD2	1:A:273:LYS:O	1.34	1.10
1:C:277:CYS:HB2	1:D:281:MET:HG3	1.33	1.09
1:C:217:TYR:CD2	1:C:274:GLN:NE2	2.21	1.08
1:D:217:TYR:HA	1:D:218:SER:CB	1.85	1.07
1:B:200:LEU:HD12	1:B:200:LEU:H	1.19	1.07
1:C:227:TRP:CE3	1:C:260:ARG:HG2	1.89	1.07
1:C:277:CYS:HB2	1:D:281:MET:CG	1.82	1.06
1:A:217:TYR:CD2	1:A:273:LYS:O	2.08	1.05
1:A:93:ALA:HB1	1:A:95:GLU:C	1.80	1.05
1:B:293:ASN:C	1:B:293:ASN:HD22	1.57	1.02
1:C:227:TRP:CZ3	1:C:260:ARG:HA	1.93	1.02
1:D:261:VAL:HG11	1:D:265:LYS:HG2	1.39	1.02
1:B:292:SER:O	1:B:293:ASN:O	1.79	1.01
1:C:227:TRP:CZ3	1:C:260:ARG:HG2	1.96	1.00
1:D:216:TYR:HB3	3:D:2031:HOH:O	1.62	0.97
1:A:93:ALA:CB	1:A:96:LEU:N	2.28	0.96
1:B:201:PRO:HG2	1:B:208:MET:HE2	1.47	0.94
1:D:217:TYR:HA	1:D:218:SER:HB3	1.46	0.94
1:A:268:SER:H	1:A:270:ILE:HD11	1.31	0.94
1:A:93:ALA:O	1:A:96:LEU:HB3	1.69	0.93
1:C:216:TYR:HD1	1:C:217:TYR:HB3	1.32	0.91
1:D:61:LEU:HB3	1:D:62:PRO:HD3	1.50	0.90
1:D:265:LYS:HA	1:D:265:LYS:CE	1.94	0.90
1:B:215:GLY:HA3	1:B:216:TYR:CZ	2.05	0.90
1:D:200:LEU:H	1:D:201:PRO:CD	1.86	0.89
1:A:93:ALA:HB3	1:A:96:LEU:HB2	1.52	0.88
1:D:261:VAL:CG1	1:D:265:LYS:HG2	2.03	0.88
1:D:56:PHE:CE2	1:D:58:HIS:O	2.26	0.88
1:B:293:ASN:OXT	1:B:293:ASN:ND2	2.07	0.87
1:D:262:ASP:HB3	1:D:263:PHE:HD1	1.40	0.87
1:B:215:GLY:HA3	1:B:216:TYR:CE1	2.08	0.87
1:D:199:THR:N	1:D:210:TYR:HH	1.72	0.86
1:B:293:ASN:C	1:B:293:ASN:ND2	2.31	0.85
1:D:61:LEU:CB	1:D:62:PRO:HD3	2.05	0.85
1:A:56:PHE:CD2	1:A:57:TRP:O	2.32	0.83
1:A:93:ALA:C	1:A:96:LEU:H	1.85	0.83
1:D:56:PHE:HE2	1:D:58:HIS:O	1.62	0.82
1:D:261:VAL:HG11	1:D:265:LYS:CG	2.09	0.82
1:A:95:GLU:HB2	1:A:98:LEU:HD22	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ALA:HB1	1:B:281:MET:SD	2.19	0.82
1:D:217:TYR:HA	1:D:218:SER:HB2	1.59	0.81
1:A:95:GLU:O	1:A:99:LYS:HG2	1.78	0.81
1:D:261:VAL:O	1:D:262:ASP:HB2	1.81	0.80
1:D:95:GLU:O	1:D:99:LYS:HG2	1.81	0.80
1:C:202:ALA:HB1	1:C:281:MET:SD	2.21	0.80
1:A:200:LEU:N	1:A:201:PRO:HD3	1.97	0.79
1:C:95:GLU:O	1:C:99:LYS:HG2	1.81	0.79
1:A:102:GLU:O	1:A:106:VAL:HG23	1.83	0.78
1:C:216:TYR:HB2	1:C:217:TYR:HB2	1.63	0.78
1:B:95:GLU:O	1:B:99:LYS:HG2	1.83	0.78
1:D:200:LEU:H	1:D:201:PRO:HD2	1.49	0.77
1:B:102:GLU:O	1:B:106:VAL:HG23	1.82	0.77
1:C:217:TYR:CD2	1:C:274:GLN:CD	2.62	0.77
1:C:217:TYR:HD2	1:C:274:GLN:NE2	1.81	0.77
1:C:277:CYS:HB2	1:D:281:MET:HG2	1.65	0.77
1:C:217:TYR:HD2	1:C:274:GLN:CD	1.94	0.76
1:D:263:PHE:CD1	1:D:263:PHE:N	2.52	0.76
1:D:102:GLU:O	1:D:106:VAL:HG23	1.84	0.76
1:B:215:GLY:HA3	1:B:216:TYR:CE2	2.21	0.75
1:C:102:GLU:O	1:C:106:VAL:HG23	1.85	0.75
1:B:199:THR:O	1:B:201:PRO:HD2	1.86	0.75
1:A:93:ALA:HB3	1:A:96:LEU:CB	2.17	0.74
1:D:263:PHE:HD1	1:D:263:PHE:N	1.85	0.74
1:A:261:VAL:HG11	1:A:270:ILE:O	1.87	0.73
1:D:216:TYR:HD2	1:D:273:LYS:O	1.71	0.73
1:B:215:GLY:HA3	1:B:216:TYR:CD1	2.24	0.73
1:A:95:GLU:CB	1:A:98:LEU:HD22	2.19	0.73
1:B:95:GLU:HB2	1:B:98:LEU:HD22	1.71	0.72
1:C:216:TYR:HD1	1:C:217:TYR:CB	2.02	0.72
1:C:217:TYR:CE2	1:C:274:GLN:NE2	2.58	0.71
1:D:61:LEU:HB3	1:D:62:PRO:CD	2.10	0.71
1:A:268:SER:H	1:A:270:ILE:CD1	2.03	0.71
1:C:227:TRP:HE3	1:C:260:ARG:HG2	1.52	0.71
1:B:200:LEU:HD12	1:B:200:LEU:N	1.98	0.71
1:D:266:ASP:CG	1:D:266:ASP:O	2.31	0.70
1:D:200:LEU:N	1:D:201:PRO:CD	2.51	0.70
1:D:61:LEU:CB	1:D:62:PRO:CD	2.67	0.70
1:B:201:PRO:CG	1:B:208:MET:HE2	2.21	0.70
1:C:273:LYS:HB2	1:D:204:ALA:HB2	1.72	0.69
1:D:217:TYR:CA	1:D:218:SER:CB	2.63	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:PHE:O	1:C:128:TYR:HB2	1.92	0.69
1:D:199:THR:N	1:D:210:TYR:CZ	2.61	0.69
1:B:199:THR:C	1:B:201:PRO:HD3	2.18	0.68
1:C:269:ALA:HA	1:C:272:LYS:HD2	1.75	0.68
1:B:98:LEU:O	1:B:102:GLU:HB2	1.93	0.68
1:B:54:ARG:O	1:B:55:PHE:HB2	1.93	0.67
1:D:95:GLU:HB2	1:D:98:LEU:HD22	1.77	0.67
1:D:265:LYS:HE2	1:D:265:LYS:C	2.19	0.67
1:A:98:LEU:O	1:A:102:GLU:HB2	1.93	0.67
1:A:93:ALA:CB	1:A:96:LEU:CA	2.72	0.66
1:D:98:LEU:O	1:D:102:GLU:HB2	1.95	0.66
1:D:262:ASP:HB3	1:D:263:PHE:CD1	2.26	0.66
1:D:262:ASP:CG	1:D:262:ASP:O	2.33	0.66
1:B:266:ASP:N	1:B:267:PRO:CD	2.59	0.66
1:B:199:THR:HA	3:B:2017:HOH:O	1.96	0.66
1:B:292:SER:O	1:B:293:ASN:C	2.37	0.66
1:C:227:TRP:CH2	1:C:260:ARG:HA	2.31	0.65
1:D:216:TYR:HE2	1:D:273:LYS:H	1.43	0.65
1:A:93:ALA:C	1:A:95:GLU:N	2.52	0.65
1:B:200:LEU:N	1:B:201:PRO:HD3	2.11	0.65
1:D:101:HIS:O	1:D:105:THR:HG23	1.97	0.65
1:C:216:TYR:CD1	1:C:217:TYR:HB3	2.23	0.65
1:C:95:GLU:HB2	1:C:98:LEU:HD22	1.79	0.65
1:D:266:ASP:O	1:D:266:ASP:OD2	2.14	0.64
1:C:277:CYS:CB	1:D:281:MET:CG	2.70	0.64
1:A:93:ALA:O	1:A:96:LEU:N	2.27	0.64
1:C:98:LEU:O	1:C:102:GLU:HB2	1.97	0.64
1:B:199:THR:CA	3:B:2017:HOH:O	2.45	0.63
1:D:262:ASP:O	1:D:262:ASP:OD1	2.16	0.63
1:B:123:GLU:O	1:B:123:GLU:HG2	1.98	0.63
1:A:272:LYS:O	1:A:273:LYS:HB3	1.98	0.63
1:D:261:VAL:HG11	1:D:265:LYS:CD	2.28	0.63
1:D:101:HIS:O	1:D:105:THR:CG2	2.47	0.63
1:C:61:LEU:HG	1:C:65:ARG:HD2	1.80	0.62
1:B:199:THR:C	1:B:201:PRO:CD	2.73	0.62
1:B:266:ASP:N	1:B:267:PRO:HD3	2.15	0.62
1:B:58:HIS:O	1:B:63:GLU:OE1	2.19	0.61
1:D:261:VAL:O	1:D:262:ASP:CB	2.49	0.61
1:D:217:TYR:CA	1:D:218:SER:HB3	2.25	0.61
1:A:93:ALA:HB3	1:A:96:LEU:CA	2.29	0.61
1:B:215:GLY:HA3	1:B:216:TYR:CD2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:263:PHE:C	1:D:264:CYS:SG	2.84	0.60
1:B:127:ILE:HD13	1:D:130:TYR:CE2	2.37	0.60
1:D:57:TRP:HE3	1:D:57:TRP:HA	1.67	0.60
1:A:38:LYS:HE2	3:A:2053:HOH:O	2.02	0.59
1:B:95:GLU:CB	1:B:98:LEU:HD22	2.32	0.59
1:D:287:HIS:HE1	3:D:2053:HOH:O	1.83	0.59
1:D:95:GLU:CB	1:D:98:LEU:HD22	2.33	0.59
1:C:216:TYR:HE1	1:C:274:GLN:HA	1.68	0.59
1:D:267:PRO:C	1:D:269:ALA:H	2.11	0.59
1:C:227:TRP:CZ3	1:C:260:ARG:CA	2.79	0.59
1:D:216:TYR:CD2	1:D:273:LYS:O	2.55	0.58
1:D:57:TRP:HA	1:D:57:TRP:CE3	2.37	0.58
1:B:55:PHE:CE2	1:B:131:ASP:HB2	2.38	0.58
1:C:95:GLU:CB	1:C:98:LEU:HD22	2.33	0.58
1:D:199:THR:N	1:D:210:TYR:OH	2.37	0.58
1:D:202:ALA:HB1	1:D:281:MET:SD	2.42	0.58
1:B:261:VAL:C	1:B:267:PRO:HG2	2.27	0.58
1:A:76:ARG:HD3	3:A:2014:HOH:O	2.02	0.58
1:C:273:LYS:HB2	1:D:204:ALA:CB	2.34	0.58
1:C:227:TRP:HZ3	1:C:260:ARG:HG2	1.65	0.57
1:D:235:MET:HE2	1:D:235:MET:HA	1.85	0.57
1:B:215:GLY:HA3	1:B:216:TYR:CG	2.40	0.56
1:C:216:TYR:CD1	1:C:217:TYR:CB	2.87	0.56
1:C:227:TRP:CZ3	1:C:260:ARG:CG	2.81	0.56
1:B:272:LYS:O	1:B:273:LYS:HD3	2.06	0.55
1:A:209:CYS:HB3	3:A:2039:HOH:O	2.05	0.55
1:D:99:LYS:HB3	1:D:99:LYS:HZ2	1.72	0.55
1:B:100:ILE:HG22	1:B:101:HIS:N	2.21	0.55
1:A:210:TYR:HB3	1:A:212:VAL:O	2.06	0.55
1:D:293:ASN:OD1	1:D:293:ASN:C	2.48	0.55
1:C:227:TRP:HZ3	1:C:260:ARG:HA	1.63	0.55
1:C:64:ARG:HH11	1:C:64:ARG:HG2	1.72	0.55
1:A:261:VAL:HG22	1:A:267:PRO:HB3	1.89	0.54
1:B:199:THR:O	1:B:201:PRO:CD	2.56	0.54
1:C:33:PRO:HG3	1:D:239:TYR:CZ	2.43	0.54
1:B:99:LYS:O	1:B:103:VAL:HG22	2.08	0.54
1:B:200:LEU:N	1:B:201:PRO:CD	2.71	0.54
1:A:202:ALA:HB1	1:A:206:PHE:CG	2.43	0.54
1:C:211:SER:O	1:C:276:PRO:HG3	2.08	0.53
1:A:200:LEU:N	1:A:201:PRO:CD	2.67	0.53
1:B:127:ILE:HD13	1:D:130:TYR:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ALA:HB1	1:B:281:MET:HE1	1.90	0.53
1:C:61:LEU:HG	1:C:65:ARG:CD	2.39	0.53
1:D:267:PRO:O	1:D:269:ALA:N	2.42	0.53
1:B:55:PHE:HE2	1:B:131:ASP:CG	2.16	0.53
1:D:217:TYR:CD1	1:D:218:SER:N	2.77	0.53
1:C:54:ARG:HG3	1:C:55:PHE:CD2	2.44	0.53
1:C:256:VAL:O	1:C:260:ARG:HG3	2.08	0.52
1:A:231:ASP:OD2	1:A:259:ARG:HD2	2.09	0.52
1:A:56:PHE:CE2	1:A:57:TRP:O	2.63	0.52
1:B:202:ALA:HB1	1:B:281:MET:CE	2.39	0.52
1:B:215:GLY:CA	1:B:216:TYR:CD2	2.93	0.52
1:C:292:SER:OG	1:C:293:ASN:C	2.52	0.52
1:B:203:GLY:H	1:B:281:MET:CE	2.23	0.52
1:B:269:ALA:HB1	1:B:272:LYS:HD2	1.91	0.52
1:A:93:ALA:O	1:A:96:LEU:CB	2.52	0.51
1:A:95:GLU:HA	1:A:98:LEU:HD13	1.91	0.51
1:B:133:LYS:HE3	1:B:198:TYR:HB2	1.92	0.51
1:A:93:ALA:HB1	1:A:96:LEU:CA	2.35	0.50
1:B:203:GLY:H	1:B:281:MET:HE1	1.75	0.50
1:D:216:TYR:HE2	1:D:273:LYS:N	2.09	0.50
1:B:270:ILE:HD12	1:B:270:ILE:C	2.36	0.50
1:C:277:CYS:CB	1:D:281:MET:HG2	2.35	0.50
1:D:200:LEU:H	1:D:201:PRO:HD3	1.72	0.50
1:C:216:TYR:CE1	1:C:274:GLN:HA	2.47	0.50
1:C:210:TYR:O	1:C:276:PRO:HB3	2.12	0.50
1:D:60:THR:OG1	1:D:62:PRO:HD2	2.11	0.50
1:D:200:LEU:N	1:D:201:PRO:HD3	2.26	0.50
1:D:200:LEU:HB3	1:D:201:PRO:HD3	1.94	0.50
1:B:55:PHE:CE2	1:B:131:ASP:CG	2.89	0.50
1:D:267:PRO:C	1:D:269:ALA:N	2.66	0.50
1:A:93:ALA:C	1:A:96:LEU:N	2.65	0.50
1:D:262:ASP:C	1:D:263:PHE:HD1	2.20	0.49
1:C:57:TRP:O	1:C:58:HIS:HB2	2.12	0.49
1:C:257:SER:O	1:C:261:VAL:HG23	2.11	0.49
1:D:54:ARG:O	1:D:55:PHE:HB2	2.12	0.49
1:C:217:TYR:CE2	1:C:274:GLN:CD	2.91	0.49
1:A:268:SER:N	1:A:270:ILE:HD11	2.13	0.48
1:A:200:LEU:HD22	1:A:210:TYR:OH	2.13	0.48
1:B:215:GLY:CA	1:B:216:TYR:CG	2.97	0.48
1:D:58:HIS:O	1:D:63:GLU:OE1	2.31	0.48
1:B:200:LEU:H	1:B:200:LEU:CD1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LYS:O	1:C:103:VAL:HG22	2.13	0.48
1:C:235:MET:HA	1:C:235:MET:HE2	1.96	0.48
1:B:215:GLY:C	1:B:216:TYR:CG	2.92	0.48
1:A:100:ILE:O	1:A:101:HIS:C	2.57	0.47
1:B:95:GLU:HA	1:B:98:LEU:HD13	1.96	0.47
1:C:238:LYS:HB2	1:C:238:LYS:HE3	1.57	0.47
1:D:76:ARG:HD3	3:D:2011:HOH:O	2.14	0.47
1:D:261:VAL:HG13	1:D:262:ASP:H	1.80	0.47
1:A:99:LYS:O	1:A:103:VAL:HG22	2.15	0.47
1:A:227:TRP:HB2	3:A:2052:HOH:O	2.14	0.47
1:B:59:LEU:HD13	1:B:59:LEU:HA	1.75	0.47
1:B:198:TYR:CD2	1:B:198:TYR:O	2.67	0.47
1:B:215:GLY:CA	1:B:216:TYR:CE2	2.96	0.47
1:A:99:LYS:HB3	1:A:99:LYS:HZ2	1.79	0.47
1:A:100:ILE:HG22	1:A:101:HIS:N	2.29	0.47
1:B:55:PHE:CZ	1:D:127:ILE:HG21	2.50	0.47
1:D:261:VAL:HG11	1:D:265:LYS:HD2	1.96	0.47
1:A:97:LEU:HA	1:A:100:ILE:HB	1.96	0.46
1:B:293:ASN:OXT	1:B:293:ASN:CG	2.58	0.46
1:C:216:TYR:CE1	1:C:274:GLN:HG2	2.51	0.46
1:B:261:VAL:HB	1:B:267:PRO:CB	2.46	0.46
1:C:95:GLU:HA	1:C:98:LEU:HD13	1.97	0.46
1:A:123:GLU:O	1:A:123:GLU:HG2	2.14	0.46
1:D:134:ILE:HD13	1:D:134:ILE:N	2.30	0.46
1:B:61:LEU:N	1:B:62:PRO:HD2	2.30	0.46
1:A:272:LYS:O	1:A:273:LYS:HD2	2.15	0.46
1:A:93:ALA:CB	1:A:96:LEU:CB	2.91	0.46
1:D:257:SER:HA	1:D:274:GLN:O	2.15	0.45
1:B:99:LYS:HZ2	1:B:99:LYS:HB3	1.81	0.45
1:A:95:GLU:HA	1:A:98:LEU:HD22	1.99	0.45
1:A:95:GLU:CA	1:A:98:LEU:HD22	2.46	0.45
1:A:268:SER:N	1:A:270:ILE:CD1	2.75	0.45
1:B:100:ILE:O	1:B:103:VAL:HG23	2.17	0.45
1:D:238:LYS:HE3	1:D:238:LYS:HB2	1.69	0.45
1:D:99:LYS:HB3	1:D:99:LYS:NZ	2.30	0.45
1:A:61:LEU:N	1:A:62:PRO:HD2	2.32	0.45
1:B:55:PHE:HE2	1:B:131:ASP:HB2	1.81	0.45
1:B:100:ILE:O	1:B:101:HIS:C	2.59	0.45
1:D:95:GLU:HA	1:D:98:LEU:HD13	1.98	0.45
1:D:202:ALA:HB1	1:D:281:MET:HE1	1.97	0.45
1:B:64:ARG:HG2	1:B:64:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LEU:N	1:C:62:PRO:HD2	2.32	0.45
1:A:261:VAL:CG1	1:A:270:ILE:O	2.61	0.45
1:B:199:THR:C	3:B:2017:HOH:O	2.60	0.45
1:B:209:CYS:HB3	3:B:2022:HOH:O	2.17	0.45
1:B:238:LYS:HE3	1:B:238:LYS:HB2	1.62	0.45
1:B:133:LYS:HE3	1:B:198:TYR:CB	2.47	0.45
1:D:97:LEU:HA	1:D:100:ILE:HB	1.99	0.45
1:A:239:TYR:CZ	1:B:33:PRO:HG3	2.52	0.44
1:C:97:LEU:HA	1:C:100:ILE:HB	1.99	0.44
1:C:89:ASN:C	1:C:89:ASN:OD1	2.61	0.44
1:D:67:THR:OG1	1:D:121:HIS:CE1	2.70	0.44
1:B:215:GLY:CA	1:B:216:TYR:CD1	2.97	0.44
1:B:54:ARG:O	1:B:55:PHE:CB	2.61	0.44
1:C:61:LEU:CD1	1:C:64:ARG:NH2	2.81	0.44
1:C:61:LEU:CG	1:C:65:ARG:HD2	2.46	0.44
1:B:261:VAL:HG21	1:B:269:ALA:O	2.18	0.43
1:D:56:PHE:O	1:D:57:TRP:CE3	2.71	0.43
1:D:199:THR:O	1:D:199:THR:HG22	2.16	0.43
1:A:216:TYR:N	1:A:216:TYR:CD1	2.85	0.43
1:A:144:LYS:O	1:A:145:GLY:C	2.60	0.43
1:B:55:PHE:CE2	1:B:131:ASP:CB	3.02	0.43
1:B:89:ASN:OD1	1:B:89:ASN:C	2.61	0.43
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.71	0.43
1:B:101:HIS:O	1:B:104:SER:HB2	2.18	0.43
1:D:217:TYR:HD1	1:D:218:SER:N	2.17	0.43
1:A:201:PRO:CD	1:A:201:PRO:O	2.67	0.42
1:C:219:HIS:HB2	1:C:227:TRP:CZ3	2.54	0.42
1:B:202:ALA:CB	1:B:281:MET:SD	3.02	0.42
1:C:281:MET:HG3	1:D:277:CYS:HB2	2.00	0.42
1:A:235:MET:HA	1:A:235:MET:HE2	2.01	0.42
1:D:95:GLU:HA	1:D:98:LEU:HB2	2.01	0.42
1:A:61:LEU:CD1	1:A:64:ARG:NH2	2.83	0.42
1:C:265:LYS:HE2	1:C:265:LYS:HB2	1.83	0.42
1:B:97:LEU:HA	1:B:100:ILE:HB	2.01	0.42
1:C:61:LEU:HB3	1:C:62:PRO:HD3	2.02	0.42
1:C:120:SER:H	1:C:161:GLN:HE21	1.67	0.42
1:D:99:LYS:O	1:D:103:VAL:HG22	2.19	0.42
1:A:54:ARG:O	1:A:55:PHE:HB2	2.20	0.42
1:C:291:LYS:HB3	1:C:291:LYS:HE3	1.90	0.42
1:D:100:ILE:O	1:D:103:VAL:HG23	2.20	0.42
1:A:64:ARG:HH11	1:A:64:ARG:HG2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ARG:HG2	1:D:64:ARG:HH11	1.85	0.41
1:D:48:LEU:C	1:D:48:LEU:HD23	2.45	0.41
1:D:50:PHE:HD1	1:D:88:PHE:CE1	2.39	0.41
1:B:61:LEU:CD1	1:B:64:ARG:NH2	2.83	0.41
1:D:214:GLU:HG3	1:D:214:GLU:O	2.21	0.41
1:A:99:LYS:HB3	1:A:99:LYS:NZ	2.35	0.41
1:B:55:PHE:HZ	1:D:127:ILE:HG13	1.85	0.41
1:C:216:TYR:CB	1:C:217:TYR:HB2	2.42	0.41
1:D:40:ASP:OD1	3:D:2005:HOH:O	2.22	0.41
1:D:268:SER:O	1:D:272:LYS:HE3	2.20	0.41
1:A:61:LEU:HB3	1:A:62:PRO:HD3	2.04	0.41
1:C:211:SER:HA	1:C:228:TYR:CD1	2.56	0.41
1:B:115:VAL:HG22	1:B:157:ILE:HB	2.03	0.40
1:C:95:GLU:HA	1:C:98:LEU:HB2	2.02	0.40
1:D:199:THR:O	1:D:199:THR:CG2	2.66	0.40
1:A:95:GLU:HA	1:A:98:LEU:HB2	2.03	0.40
1:A:238:LYS:HB2	1:A:238:LYS:HE3	1.70	0.40
1:C:59:LEU:HD13	1:C:59:LEU:HA	1.74	0.40
1:D:235:MET:HE2	1:D:235:MET:CA	2.50	0.40
1:A:41:HIS:HD2	1:A:112:ASP:OD1	2.05	0.40
1:A:87:CYS:HB3	3:A:2011:HOH:O	2.21	0.40
1:B:50:PHE:HD1	1:B:88:PHE:CE1	2.40	0.40
1:B:235:MET:HE2	1:B:235:MET:HA	2.03	0.40
1:B:266:ASP:N	1:B:266:ASP:OD1	2.54	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ARG:NE	1:D:61:LEU:CD2[1_655]	1.53	0.67
1:C:220:ARG:CD	1:D:61:LEU:CD2[1_655]	1.76	0.44
1:A:98:LEU:CD2	1:B:101:HIS:CD2[1_655]	1.87	0.33
1:A:101:HIS:CD2	1:B:98:LEU:CD2[1_655]	2.03	0.17
1:C:102:GLU:OE1	1:C:270:ILE:O[2_545]	2.06	0.14
1:B:238:LYS:NZ	1:D:292:SER:OG[1_554]	2.08	0.12
1:A:98:LEU:CD2	1:B:101:HIS:NE2[1_655]	2.18	0.02
1:C:64:ARG:NH1	1:D:264:CYS:CB[1_655]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	218/293 (74%)	200 (92%)	15 (7%)	3 (1%)	9	3
1	B	221/293 (75%)	208 (94%)	12 (5%)	1 (0%)	24	16
1	C	223/293 (76%)	207 (93%)	13 (6%)	3 (1%)	9	3
1	D	226/293 (77%)	204 (90%)	19 (8%)	3 (1%)	9	3
All	All	888/1172 (76%)	819 (92%)	59 (7%)	10 (1%)	11	4

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	201	PRO
1	C	273	LYS
1	D	200	LEU
1	D	267	PRO
1	C	274	GLN
1	D	266	ASP
1	A	59	LEU
1	A	93	ALA
1	C	122	GLY
1	A	215	GLY

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	195/255 (76%)	183 (94%)	12 (6%)	16	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	198/255 (78%)	187 (94%)	11 (6%)	19	8
1	C	198/255 (78%)	186 (94%)	12 (6%)	17	7
1	D	201/255 (79%)	184 (92%)	17 (8%)	10	3
All	All	792/1020 (78%)	740 (93%)	52 (7%)	15	5

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	92	LYS
1	A	99	LYS
1	A	100	ILE
1	A	103	VAL
1	A	105	THR
1	A	123	GLU
1	A	144	LYS
1	A	255	LYS
1	A	261	VAL
1	A	268	SER
1	A	270	ILE
1	B	57	TRP
1	B	59	LEU
1	B	99	LYS
1	B	100	ILE
1	B	103	VAL
1	B	105	THR
1	B	123	GLU
1	B	200	LEU
1	B	255	LYS
1	B	266	ASP
1	B	293	ASN
1	C	59	LEU
1	C	65	ARG
1	C	71	ARG
1	C	99	LYS
1	C	100	ILE
1	C	103	VAL
1	C	105	THR
1	C	255	LYS
1	C	257	SER
1	C	273	LYS

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Mol	Chain	Res	Type
1	C	277	CYS
1	C	293	ASN
1	D	57	TRP
1	D	59	LEU
1	D	60	THR
1	D	61	LEU
1	D	99	LYS
1	D	100	ILE
1	D	103	VAL
1	D	105	THR
1	D	123	GLU
1	D	164	ARG
1	D	216	TYR
1	D	255	LYS
1	D	261	VAL
1	D	262	ASP
1	D	263	PHE
1	D	265	LYS
1	D	293	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
1	A	51	ASN
1	A	161	GLN
1	B	51	ASN
1	B	137	GLN
1	B	161	GLN
1	B	287	HIS
1	B	293	ASN
1	C	51	ASN
1	C	121	HIS
1	D	161	GLN
1	D	287	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	D	1294	-	4,4,4	0.92	0	6,6,6	0.47	0

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	224/293 (76%)	-0.98	0 100 100	11, 32, 92, 118	0
1	B	227/293 (77%)	-0.90	0 100 100	12, 33, 97, 123	0
1	C	227/293 (77%)	-0.90	0 100 100	16, 35, 97, 118	0
1	D	230/293 (78%)	-0.89	0 100 100	16, 32, 99, 119	0
All	All	908/1172 (77%)	-0.92	0 100 100	11, 34, 99, 123	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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	PO4	D	1294	5/5	0.97	0.07	123,125,131,136	0

6.5 Other polymers [i](#)

There are no such residues in this entry.