



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:42 AM UTC

PDB ID : 1AAM / pdb_00001aam
Title : THE STRUCTURAL BASIS FOR THE ALTERED SUBSTRATE SPECIFICITY OF THE R292D ACTIVE SITE MUTANT OF ASPARTATE AMINOTRANSFERASE FROM E. COLI
Authors : Almo, S.C.; Smith, D.L.; Danishefsky, A.T.; Ringe, D.
Deposited on : 1993-07-13
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

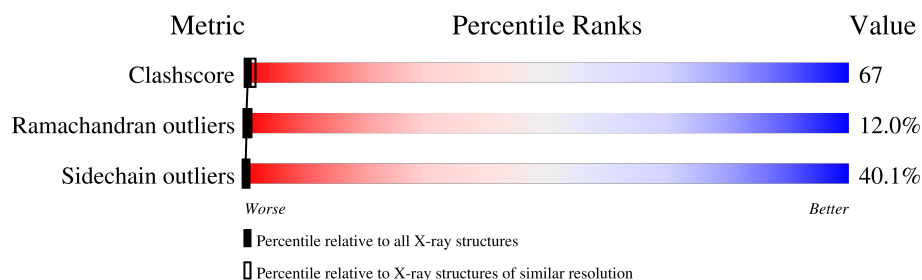
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3086 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.

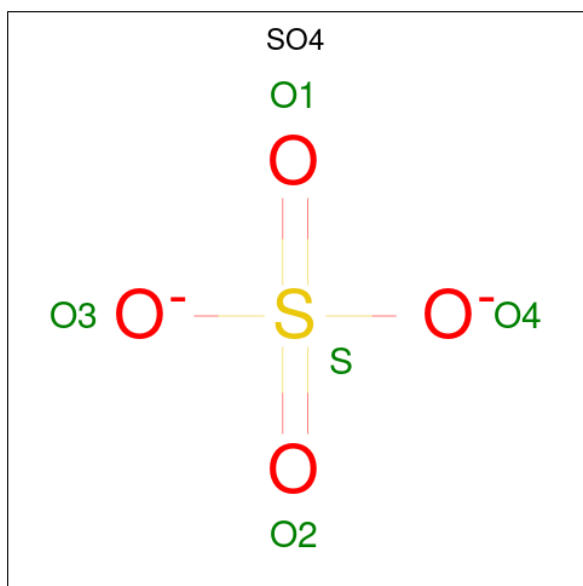
- Molecule 1 is a protein called Aspartate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	396	3081	1942	534	591	1	13	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ASP	ARG	engineered mutation	UNP P00509

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

- Molecule 1: Aspartate aminotransferase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	155.40Å 87.00Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3086	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.87	0/3117	3.15	429/4223 (10.2%)

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	6

There are no bond length outliers.

All (429) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	14	PHE	CA-CB-CG	23.42	137.22	113.80
1	A	114	GLY	N-CA-C	19.16	137.28	114.48
1	A	41	ILE	CA-C-O	17.54	132.41	120.66
1	A	171	PHE	CA-CB-CG	17.33	131.13	113.80
1	A	25	ILE	CA-C-N	16.78	154.41	121.18
1	A	25	ILE	C-N-CA	16.78	154.41	121.18
1	A	124	ASP	CA-CB-CG	16.44	129.04	112.60
1	A	292	ASP	CA-CB-CG	16.01	128.61	112.60
1	A	206	TRP	CA-CB-CG	14.65	141.44	113.60
1	A	137	VAL	N-CA-C	13.63	137.70	109.34
1	A	377	PHE	CA-CB-CG	13.20	127.00	113.80
1	A	193	CYS	CA-C-N	12.99	146.36	121.54
1	A	193	CYS	C-N-CA	12.99	146.36	121.54
1	A	27	GLY	N-CA-C	-12.73	98.76	114.16
1	A	181	ALA	CA-C-N	12.60	145.60	121.54
1	A	181	ALA	C-N-CA	12.60	145.60	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ILE	N-CA-CB	12.55	131.94	111.23
1	A	190	HIS	N-CA-C	12.48	127.31	109.71
1	A	25	ILE	CA-C-O	12.43	136.31	120.78
1	A	226	TYR	N-CA-C	12.38	126.69	109.11
1	A	197	THR	N-CA-CB	11.93	127.33	110.26
1	A	39	GLY	N-CA-C	11.90	141.38	113.18
1	A	22	ALA	N-CA-C	11.68	125.73	110.43
1	A	166	ASN	N-CA-CB	11.59	129.52	110.39
1	A	17	ILE	CA-C-O	11.38	135.00	120.78
1	A	325	ASP	CA-CB-CG	11.37	123.97	112.60
1	A	330	ILE	N-CA-CB	11.14	123.24	110.65
1	A	33	ARG	N-CA-C	-10.65	99.67	111.07
1	A	366	THR	CA-C-N	10.61	141.80	121.54
1	A	366	THR	C-N-CA	10.61	141.80	121.54
1	A	334	ARG	CD-NE-CZ	10.55	139.17	124.40
1	A	109	THR	N-CA-C	10.47	126.94	109.76
1	A	37	ARG	N-CA-C	10.47	126.09	110.39
1	A	60	SER	CA-C-O	10.41	132.57	120.92
1	A	14	PHE	N-CA-C	-10.35	97.96	112.13
1	A	193	CYS	CA-C-O	10.31	132.97	120.60
1	A	108	ARG	CA-C-N	10.09	137.68	122.65
1	A	108	ARG	C-N-CA	10.09	137.68	122.65
1	A	236	ASP	CA-CB-CG	10.02	122.62	112.60
1	A	182	GLN	N-CA-C	9.89	131.86	110.80
1	A	264	ASN	N-CA-C	9.76	123.14	111.82
1	A	170	ASP	CA-CB-CG	-9.74	102.86	112.60
1	A	157	ARG	CD-NE-CZ	9.72	138.01	124.40
1	A	90	THR	N-CA-C	-9.71	100.38	110.97
1	A	276	ASP	CA-CB-CG	9.43	122.03	112.60
1	A	330	ILE	CB-CA-C	-9.39	99.76	111.87
1	A	163	ASP	CA-CB-CG	9.38	121.98	112.60
1	A	204	GLU	CB-CG-CD	9.37	128.53	112.60
1	A	224	PHE	CA-CB-CG	9.31	123.11	113.80
1	A	100	ALA	CA-C-O	-9.27	108.67	119.61
1	A	33	ARG	CA-C-O	9.14	130.42	120.82
1	A	41	ILE	CA-C-N	9.14	139.41	121.58
1	A	41	ILE	C-N-CA	9.14	139.41	121.58
1	A	241	ARG	CA-CB-CG	9.09	132.29	114.10
1	A	35	ASP	CA-CB-CG	8.98	121.58	112.60
1	A	142	TRP	N-CA-C	-8.92	92.50	108.47
1	A	393	THR	CA-C-N	8.92	128.95	119.05
1	A	393	THR	C-N-CA	8.92	128.95	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	THR	N-CA-CB	-8.85	95.91	110.52
1	A	179	ASN	CA-CB-CG	8.85	121.45	112.60
1	A	116	THR	N-CA-C	-8.85	100.16	112.45
1	A	146	LYS	N-CA-C	-8.83	102.08	113.12
1	A	342	GLN	N-CA-C	-8.80	101.77	111.36
1	A	388	ASN	CA-CB-CG	-8.79	103.81	112.60
1	A	186	VAL	CA-C-O	8.77	132.18	121.92
1	A	166	ASN	N-CA-C	-8.76	91.45	107.75
1	A	349	ASP	CA-CB-CG	8.74	121.34	112.60
1	A	15	GLU	CB-CG-CD	8.71	127.40	112.60
1	A	192	CYS	N-CA-C	-8.70	98.38	111.34
1	A	186	VAL	CA-C-N	8.67	134.82	122.77
1	A	186	VAL	C-N-CA	8.67	134.82	122.77
1	A	106	ARG	CA-CB-CG	8.62	131.34	114.10
1	A	387	VAL	N-CA-C	8.56	122.24	108.97
1	A	360	PHE	CA-C-O	8.55	129.78	120.71
1	A	392	MET	N-CA-C	8.48	123.86	113.17
1	A	181	ALA	CA-C-O	8.47	130.51	121.19
1	A	310	LEU	CA-C-N	8.39	131.52	120.28
1	A	310	LEU	C-N-CA	8.39	131.52	120.28
1	A	267	VAL	CA-C-O	8.31	129.79	120.90
1	A	100	ALA	N-CA-C	8.23	123.04	112.34
1	A	339	ASN	N-CA-C	-8.22	102.01	110.97
1	A	21	PRO	CA-C-N	8.20	134.73	120.87
1	A	21	PRO	C-N-CA	8.20	134.73	120.87
1	A	235	GLU	CB-CG-CD	8.19	126.52	112.60
1	A	204	GLU	N-CA-C	-8.18	101.95	111.03
1	A	235	GLU	N-CA-CB	8.18	123.97	110.39
1	A	241	ARG	NE-CZ-NH2	8.16	126.54	119.20
1	A	144	ASN	N-CA-C	-8.14	102.91	112.92
1	A	158	GLU	CB-CG-CD	8.13	126.43	112.60
1	A	20	ALA	CA-C-N	8.04	129.88	119.84
1	A	20	ALA	C-N-CA	8.04	129.88	119.84
1	A	145	HIS	CA-CB-CG	8.03	121.83	113.80
1	A	402	GLU	CB-CG-CD	7.99	126.17	112.60
1	A	254	SER	O-C-N	7.94	133.75	123.11
1	A	178	LEU	N-CA-C	-7.91	102.41	112.93
1	A	195	ASN	OD1-CG-ND2	-7.86	114.74	122.60
1	A	235	GLU	N-CA-C	-7.85	102.96	112.54
1	A	335	GLN	CB-CG-CD	7.84	125.93	112.60
1	A	106	ARG	N-CA-C	-7.83	103.71	113.18
1	A	242	ALA	CA-C-O	7.81	129.02	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ALA	CA-C-N	7.78	127.06	118.97
1	A	398	ALA	C-N-CA	7.78	127.06	118.97
1	A	180	GLU	CB-CG-CD	7.73	125.74	112.60
1	A	36	GLU	N-CA-C	7.72	122.33	111.52
1	A	42	ASN	CA-CB-CG	7.70	120.30	112.60
1	A	296	SER	N-CA-CB	7.66	122.36	109.87
1	A	30	ASP	CA-CB-CG	7.66	120.26	112.60
1	A	281	ASP	CA-CB-CG	7.62	120.22	112.60
1	A	283	ALA	N-CA-C	-7.60	103.11	112.38
1	A	32	PHE	N-CA-C	-7.58	104.05	113.38
1	A	89	CYS	O-C-N	7.57	132.50	122.36
1	A	368	GLU	CB-CG-CD	7.57	125.47	112.60
1	A	368	GLU	CB-CA-C	7.57	123.90	110.81
1	A	376	GLU	N-CA-C	-7.57	94.11	107.73
1	A	21	PRO	N-CA-C	7.56	128.05	112.47
1	A	28	LEU	CA-C-N	7.56	135.98	121.54
1	A	28	LEU	C-N-CA	7.56	135.98	121.54
1	A	320	GLU	CB-CG-CD	7.55	125.44	112.60
1	A	318	ILE	CB-CA-C	7.54	122.28	111.65
1	A	366	THR	CA-C-O	7.54	131.29	120.51
1	A	83	ILE	CA-C-N	7.47	127.64	119.87
1	A	83	ILE	C-N-CA	7.47	127.64	119.87
1	A	296	SER	CA-C-O	-7.47	111.82	120.49
1	A	339	ASN	N-CA-CB	7.46	120.80	109.91
1	A	265	GLU	CA-C-N	7.43	135.72	121.54
1	A	265	GLU	C-N-CA	7.43	135.72	121.54
1	A	296	SER	O-C-N	7.42	132.14	123.02
1	A	182	GLN	CA-C-N	7.42	135.70	121.54
1	A	182	GLN	C-N-CA	7.42	135.70	121.54
1	A	90	THR	CA-C-N	7.40	132.96	121.19
1	A	90	THR	C-N-CA	7.40	132.96	121.19
1	A	395	ASP	N-CA-C	-7.38	104.08	113.23
1	A	150	ASN	N-CA-C	-7.38	104.67	112.93
1	A	121	VAL	N-CA-C	-7.34	103.13	110.62
1	A	248	LYS	N-CA-CB	7.29	122.81	110.49
1	A	345	GLY	N-CA-C	7.28	130.44	113.18
1	A	59	THR	N-CA-CB	7.26	122.77	110.49
1	A	236	ASP	CB-CA-C	7.26	123.90	110.11
1	A	41	ILE	N-CA-CB	7.24	119.40	109.84
1	A	142	TRP	CB-CA-C	7.21	118.36	110.08
1	A	243	PHE	CA-CB-CG	7.19	120.99	113.80
1	A	270	CYS	N-CA-CB	7.18	124.10	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	PHE	N-CA-C	-7.17	104.80	113.97
1	A	84	PRO	N-CA-C	7.14	122.82	114.03
1	A	229	PHE	CA-CB-CG	7.08	120.88	113.80
1	A	317	ALA	N-CA-C	-7.07	103.62	111.82
1	A	181	ALA	N-CA-C	7.06	120.47	110.23
1	A	60	SER	CA-C-N	7.06	134.68	121.97
1	A	60	SER	C-N-CA	7.06	134.68	121.97
1	A	190	HIS	N-CA-CB	-7.05	102.45	110.35
1	A	75	LYS	N-CA-C	-7.04	104.62	112.57
1	A	29	ALA	N-CA-C	7.00	125.70	110.80
1	A	24	PRO	N-CA-C	6.99	126.86	112.47
1	A	105	LYS	O-C-N	6.98	131.69	122.47
1	A	127	ALA	N-CA-C	-6.95	103.31	111.03
1	A	280	VAL	CA-C-N	6.93	129.86	120.44
1	A	280	VAL	C-N-CA	6.93	129.86	120.44
1	A	114	GLY	CA-C-O	-6.92	112.45	119.37
1	A	58	LEU	CA-C-N	6.92	134.75	121.54
1	A	58	LEU	C-N-CA	6.92	134.75	121.54
1	A	381	ALA	N-CA-CB	6.88	121.94	110.59
1	A	368	GLU	CA-C-O	6.88	128.05	119.59
1	A	342	GLN	O-C-N	6.87	129.98	122.15
1	A	366	THR	CB-CA-C	6.85	124.05	110.42
1	A	349	ASP	CB-CA-C	6.85	122.21	110.77
1	A	170	ASP	N-CA-CB	6.84	121.56	110.42
1	A	104	ASP	N-CA-C	-6.83	103.62	112.23
1	A	264	ASN	N-CA-CB	-6.83	99.70	110.28
1	A	382	VAL	N-CA-C	6.83	123.54	109.34
1	A	160	ALA	N-CA-C	6.82	120.79	108.17
1	A	296	SER	N-CA-C	-6.81	98.83	109.25
1	A	192	CYS	O-C-N	6.81	128.47	121.79
1	A	13	MET	CA-C-N	6.81	132.78	122.56
1	A	13	MET	C-N-CA	6.81	132.78	122.56
1	A	220	PRO	CA-C-O	6.81	131.14	122.15
1	A	335	GLN	O-C-N	6.81	129.33	122.12
1	A	288	LYS	CA-C-N	6.80	129.28	120.44
1	A	288	LYS	C-N-CA	6.80	129.28	120.44
1	A	120	ARG	CA-C-O	6.76	127.05	119.41
1	A	369	GLN	N-CA-C	-6.75	103.70	112.68
1	A	85	GLU	O-C-N	6.75	131.42	122.30
1	A	275	ALA	N-CA-C	6.75	125.18	110.80
1	A	172	ASP	CB-CA-C	6.74	121.55	110.90
1	A	259	ASN	CA-CB-CG	6.74	119.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	MET	N-CA-C	-6.73	103.75	112.23
1	A	199	ILE	N-CA-C	6.71	119.30	109.63
1	A	120	ARG	N-CA-C	-6.69	105.25	113.41
1	A	404	ILE	N-CA-CB	6.69	122.27	111.23
1	A	155	GLU	O-C-N	6.68	131.23	123.41
1	A	386	ARG	CA-C-O	6.67	128.31	120.70
1	A	247	HIS	CA-CB-CG	-6.67	107.13	113.80
1	A	316	ARG	CD-NE-CZ	6.67	133.74	124.40
1	A	85	GLU	N-CA-C	-6.65	102.47	112.04
1	A	136	TRP	CB-CA-C	6.64	121.18	110.29
1	A	185	ASP	O-C-N	6.64	130.79	123.22
1	A	180	GLU	CA-C-N	6.64	130.13	120.71
1	A	180	GLU	C-N-CA	6.64	130.13	120.71
1	A	132	VAL	CA-C-O	6.60	127.47	120.48
1	A	386	ARG	N-CA-C	6.58	120.58	107.62
1	A	393	THR	N-CA-C	6.57	124.33	109.81
1	A	328	GLN	CA-CB-CG	6.57	127.25	114.10
1	A	44	GLY	N-CA-C	-6.54	97.68	113.18
1	A	179	ASN	OD1-CG-ND2	6.54	129.14	122.60
1	A	247	HIS	N-CA-C	6.53	124.71	110.80
1	A	357	ASN	CA-C-N	6.53	132.30	122.05
1	A	357	ASN	C-N-CA	6.53	132.30	122.05
1	A	36	GLU	CA-C-O	6.49	129.25	121.65
1	A	19	ALA	N-CA-C	-6.49	100.31	110.36
1	A	352	PHE	N-CA-C	6.48	124.59	110.80
1	A	32	PHE	CB-CA-C	6.46	120.90	109.65
1	A	188	LEU	O-C-N	6.46	131.54	123.14
1	A	106	ARG	CB-CA-C	6.46	122.80	109.95
1	A	199	ILE	CA-C-O	6.44	128.44	121.36
1	A	126	LEU	CB-CA-C	6.43	120.85	109.65
1	A	181	ALA	O-C-N	-6.43	114.97	122.87
1	A	342	GLN	N-CA-CB	6.41	119.64	110.16
1	A	101	LEU	CA-C-N	6.40	129.51	120.42
1	A	101	LEU	C-N-CA	6.40	129.51	120.42
1	A	395	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	380	TYR	N-CA-C	6.39	118.82	108.41
1	A	98	GLY	CA-C-N	6.38	130.17	121.05
1	A	98	GLY	C-N-CA	6.38	130.17	121.05
1	A	214	VAL	N-CA-C	-6.38	104.82	111.58
1	A	372	ARG	CD-NE-CZ	6.37	133.32	124.40
1	A	303	ALA	CA-C-N	6.36	129.04	120.65
1	A	303	ALA	C-N-CA	6.36	129.04	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	N-CA-CB	-6.34	100.77	111.23
1	A	343	GLU	CB-CG-CD	6.33	123.37	112.60
1	A	341	LEU	CB-CA-C	6.32	120.74	110.37
1	A	129	ASN	CA-CB-CG	6.32	118.92	112.60
1	A	172	ASP	CA-C-N	6.31	131.37	120.58
1	A	172	ASP	C-N-CA	6.31	131.37	120.58
1	A	247	HIS	CA-C-N	6.28	133.54	121.54
1	A	247	HIS	C-N-CA	6.28	133.54	121.54
1	A	357	ASN	CA-C-O	6.28	128.21	121.55
1	A	241	ARG	N-CA-C	-6.28	104.88	112.54
1	A	191	GLY	N-CA-C	6.27	128.04	113.18
1	A	226	TYR	CB-CA-C	-6.27	102.12	111.72
1	A	261	GLY	O-C-N	6.26	129.17	122.41
1	A	213	SER	N-CA-C	-6.25	105.43	114.12
1	A	179	ASN	N-CA-CB	-6.25	99.59	109.78
1	A	323	LEU	CA-C-N	6.25	128.94	120.38
1	A	323	LEU	C-N-CA	6.25	128.94	120.38
1	A	101	LEU	CA-C-O	6.25	127.15	119.97
1	A	262	LEU	N-CA-CB	-6.24	102.14	111.25
1	A	179	ASN	CB-CA-C	6.24	121.09	110.74
1	A	37	ARG	CB-CA-C	-6.22	98.18	109.45
1	A	221	LEU	N-CA-C	-6.20	99.25	108.99
1	A	376	GLU	N-CA-CB	6.19	123.59	110.29
1	A	292	ASP	CA-C-N	6.18	132.48	120.99
1	A	292	ASP	C-N-CA	6.18	132.48	120.99
1	A	386	ARG	CD-NE-CZ	6.17	133.04	124.40
1	A	108	ARG	CD-NE-CZ	6.16	133.02	124.40
1	A	400	LEU	N-CA-CB	-6.16	100.08	110.49
1	A	78	LEU	N-CA-C	-6.15	100.54	110.32
1	A	253	ALA	N-CA-C	-6.14	97.28	108.02
1	A	360	PHE	CA-C-N	6.14	132.71	121.85
1	A	360	PHE	C-N-CA	6.14	132.71	121.85
1	A	168	THR	N-CA-C	6.14	119.66	109.96
1	A	339	ASN	O-C-N	6.10	128.38	122.03
1	A	130	THR	CB-CA-C	6.10	120.53	109.37
1	A	367	LYS	N-CA-C	6.09	123.78	110.80
1	A	383	ALA	N-CA-C	6.09	123.77	110.80
1	A	33	ARG	CA-C-N	6.06	133.12	121.54
1	A	33	ARG	C-N-CA	6.06	133.12	121.54
1	A	110	ALA	N-CA-C	6.06	119.00	108.76
1	A	385	GLY	N-CA-C	-6.03	102.09	114.16
1	A	273	VAL	CB-CA-C	6.03	118.58	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	VAL	N-CA-CB	-6.03	101.29	111.23
1	A	301	HIS	CA-CB-CG	-6.02	107.78	113.80
1	A	333	MET	CA-C-O	6.02	126.69	119.10
1	A	195	ASN	CA-CB-CG	6.02	118.62	112.60
1	A	158	GLU	N-CA-C	6.01	123.60	110.80
1	A	137	VAL	N-CA-CB	-5.99	101.36	111.23
1	A	285	SER	N-CA-C	-5.98	105.09	112.38
1	A	350	PHE	CA-C-O	5.97	126.29	119.18
1	A	297	ASN	CA-CB-CG	5.96	118.56	112.60
1	A	330	ILE	O-C-N	5.96	128.32	121.94
1	A	111	GLN	N-CA-CB	5.96	119.47	109.94
1	A	209	LEU	CB-CA-C	5.96	120.35	109.99
1	A	402	GLU	N-CA-C	-5.94	104.78	112.68
1	A	94	LEU	N-CA-C	5.90	118.22	111.02
1	A	152	ALA	N-CA-CB	5.90	122.71	112.27
1	A	86	PHE	CA-CB-CG	-5.89	107.91	113.80
1	A	207	GLN	CA-CB-CG	5.89	125.88	114.10
1	A	404	ILE	CB-CG1-CD1	5.88	126.15	113.80
1	A	105	LYS	N-CA-C	-5.87	104.05	111.92
1	A	197	THR	O-C-N	5.85	129.59	122.75
1	A	294	ASN	N-CA-CB	5.84	120.36	110.49
1	A	235	GLU	O-C-N	5.84	130.25	122.43
1	A	368	GLU	CA-CB-CG	5.84	125.78	114.10
1	A	116	THR	CA-C-O	5.83	127.12	120.00
1	A	309	ILE	N-CA-CB	5.83	117.24	110.65
1	A	111	GLN	CA-CB-CG	5.80	125.70	114.10
1	A	41	ILE	O-C-N	-5.80	116.85	122.94
1	A	372	ARG	CA-C-O	5.78	128.78	120.51
1	A	111	GLN	OE1-CD-NE2	-5.76	116.83	122.60
1	A	50	ASP	N-CA-C	5.76	118.41	109.60
1	A	178	LEU	CA-C-N	5.76	129.46	120.82
1	A	178	LEU	C-N-CA	5.76	129.46	120.82
1	A	179	ASN	CA-C-N	5.73	132.48	121.54
1	A	179	ASN	C-N-CA	5.73	132.48	121.54
1	A	146	LYS	CA-C-N	5.71	128.19	120.65
1	A	146	LYS	C-N-CA	5.71	128.19	120.65
1	A	141	SER	CA-CB-OG	5.71	122.52	111.10
1	A	25	ILE	O-C-N	-5.70	115.44	122.57
1	A	304	SER	N-CA-C	-5.69	104.77	110.97
1	A	301	HIS	N-CA-C	5.69	122.92	110.80
1	A	350	PHE	CA-C-N	5.66	132.35	121.54
1	A	350	PHE	C-N-CA	5.66	132.35	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	PRO	CA-C-O	5.65	128.23	120.03
1	A	329	ARG	CD-NE-CZ	5.64	132.30	124.40
1	A	374	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	A	25	ILE	CB-CA-C	-5.64	102.04	111.29
1	A	93	LEU	CA-C-N	5.64	128.63	120.79
1	A	93	LEU	C-N-CA	5.64	128.63	120.79
1	A	393	THR	CA-CB-OG1	-5.63	101.15	109.60
1	A	300	ALA	N-CA-C	5.63	118.50	111.24
1	A	242	ALA	N-CA-C	-5.63	105.05	111.07
1	A	180	GLU	N-CA-C	5.62	122.78	110.80
1	A	187	VAL	CA-C-O	5.62	127.63	121.67
1	A	77	TYR	N-CA-CB	5.62	118.83	109.56
1	A	88	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	272	LEU	N-CA-C	-5.61	100.10	109.24
1	A	45	ILE	N-CA-C	5.61	118.58	113.20
1	A	316	ARG	N-CA-C	-5.61	106.61	113.50
1	A	339	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	A	211	GLN	CB-CG-CD	5.58	122.09	112.60
1	A	198	GLY	CA-C-N	5.58	127.97	120.50
1	A	198	GLY	C-N-CA	5.58	127.97	120.50
1	A	264	ASN	CA-CB-CG	5.58	118.17	112.60
1	A	52	THR	N-CA-C	-5.57	105.26	113.61
1	A	372	ARG	N-CA-C	-5.56	98.95	110.80
1	A	208	THR	CA-CB-CG2	5.56	119.95	110.50
1	A	90	THR	CA-C-O	5.54	126.82	121.00
1	A	190	HIS	CA-C-N	5.54	132.28	121.41
1	A	190	HIS	C-N-CA	5.54	132.28	121.41
1	A	156	VAL	CB-CA-C	5.53	119.92	111.68
1	A	45	ILE	N-CA-CB	-5.52	104.22	112.67
1	A	56	PRO	CA-C-N	5.52	128.66	122.59
1	A	56	PRO	C-N-CA	5.52	128.66	122.59
1	A	267	VAL	N-CA-C	5.50	115.61	108.35
1	A	322	GLU	CG-CD-OE2	5.50	131.04	118.40
1	A	171	PHE	O-C-N	5.49	129.12	122.48
1	A	166	ASN	CA-C-N	5.48	132.01	121.54
1	A	166	ASN	C-N-CA	5.48	132.01	121.54
1	A	126	LEU	N-CA-CB	-5.47	102.37	110.53
1	A	99	SER	CA-C-N	5.47	129.44	120.63
1	A	99	SER	C-N-CA	5.47	129.44	120.63
1	A	239	GLY	N-CA-C	-5.46	100.25	113.18
1	A	162	TYR	CA-CB-CG	5.44	123.69	113.90
1	A	357	ASN	CB-CA-C	5.44	119.35	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASN	CA-C-O	5.43	124.75	119.22
1	A	142	TRP	CA-C-N	5.42	126.61	119.84
1	A	142	TRP	C-N-CA	5.42	126.61	119.84
1	A	155	GLU	N-CA-CB	5.42	120.94	111.13
1	A	233	LEU	N-CA-CB	5.42	119.64	110.49
1	A	262	LEU	CA-C-N	5.42	128.94	120.82
1	A	262	LEU	C-N-CA	5.42	128.94	120.82
1	A	172	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	276	ASP	CA-C-O	5.40	128.23	120.51
1	A	208	THR	N-CA-CB	-5.38	101.36	110.41
1	A	127	ALA	O-C-N	5.37	127.83	122.03
1	A	26	LEU	N-CA-C	5.35	119.43	113.01
1	A	106	ARG	NH1-CZ-NH2	-5.34	112.35	119.30
1	A	106	ARG	CD-NE-CZ	5.34	131.87	124.40
1	A	125	PHE	CA-C-O	5.33	125.84	119.60
1	A	37	ARG	N-CA-CB	-5.33	102.42	109.78
1	A	223	ASP	N-CA-CB	5.33	119.07	110.65
1	A	16	ASN	CB-CA-C	5.32	119.28	109.71
1	A	208	THR	CA-CB-OG1	-5.29	101.66	109.60
1	A	393	THR	N-CA-CB	-5.29	100.96	110.37
1	A	326	MET	N-CA-C	-5.29	106.09	112.54
1	A	322	GLU	CB-CG-CD	5.29	121.59	112.60
1	A	127	ALA	N-CA-CB	5.28	117.63	109.98
1	A	265	GLU	N-CA-C	5.27	119.69	113.16
1	A	138	SER	N-CA-CB	5.26	119.39	110.49
1	A	267	VAL	CA-C-N	5.26	129.09	120.51
1	A	267	VAL	C-N-CA	5.26	129.09	120.51
1	A	326	MET	CA-C-O	5.26	125.85	119.38
1	A	200	ASP	O-C-N	5.26	125.08	121.71
1	A	332	ARG	CD-NE-CZ	5.25	131.76	124.40
1	A	266	ARG	CA-C-O	5.23	127.98	120.51
1	A	332	ARG	CA-C-O	5.23	126.08	120.70
1	A	36	GLU	CA-C-N	5.22	132.13	121.48
1	A	36	GLU	C-N-CA	5.22	132.13	121.48
1	A	273	VAL	N-CA-CB	5.22	118.51	112.40
1	A	331	GLN	CA-C-N	5.22	127.54	120.44
1	A	331	GLN	C-N-CA	5.22	127.54	120.44
1	A	150	ASN	N-CA-CB	5.21	117.76	110.56
1	A	287	MET	CA-C-O	5.21	125.94	119.79
1	A	197	THR	CA-C-O	-5.21	116.14	121.87
1	A	332	ARG	CA-C-N	5.21	130.67	120.99
1	A	332	ARG	C-N-CA	5.21	130.67	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	158	GLU	CG-CD-OE2	5.21	130.37	118.40
1	A	306	VAL	CB-CA-C	5.21	118.99	111.65
1	A	14	PHE	CB-CA-C	5.18	119.01	110.83
1	A	357	ASN	OD1-CG-ND2	-5.17	117.43	122.60
1	A	220	PRO	N-CA-C	5.16	118.83	111.13
1	A	203	LEU	N-CA-CB	5.16	118.28	110.28
1	A	89	CYS	N-CA-C	-5.15	107.54	113.88
1	A	246	MET	CB-CA-C	-5.15	102.70	110.83
1	A	130	THR	CA-C-O	5.14	126.97	121.16
1	A	111	GLN	CB-CG-CD	5.14	121.33	112.60
1	A	200	ASP	N-CA-C	5.13	116.56	108.55
1	A	35	ASP	CA-C-N	5.13	129.47	122.34
1	A	35	ASP	C-N-CA	5.13	129.47	122.34
1	A	106	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	284	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	60	SER	CA-CB-OG	5.09	121.28	111.10
1	A	98	GLY	N-CA-C	-5.09	101.13	113.18
1	A	17	ILE	CA-C-N	5.08	130.97	122.73
1	A	17	ILE	C-N-CA	5.08	130.97	122.73
1	A	231	ARG	N-CA-CB	5.08	119.07	110.49
1	A	311	SER	N-CA-C	5.07	116.81	111.28
1	A	271	THR	CA-C-O	5.07	125.81	120.54
1	A	121	VAL	CB-CA-C	5.06	118.97	112.14
1	A	351	SER	N-CA-C	5.05	121.57	110.80
1	A	51	GLU	CA-CB-CG	5.05	124.20	114.10
1	A	256	TYR	CA-C-O	5.05	124.74	118.43
1	A	194	HIS	N-CA-C	5.04	121.54	110.80
1	A	252	VAL	CB-CA-C	5.04	118.09	110.63
1	A	285	SER	N-CA-CB	5.03	118.88	110.32
1	A	90	THR	CA-CB-CG2	5.03	119.05	110.50
1	A	331	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	178	LEU	CA-C-O	5.02	126.84	120.07
1	A	265	GLU	N-CA-CB	5.01	118.10	110.44
1	A	75	LYS	N-CA-CB	5.00	118.82	110.91
1	A	292	ASP	CA-C-O	5.00	126.53	120.92

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	ARG	Sidechain
1	A	134	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	231	ARG	Sidechain
1	A	33	ARG	Sidechain
1	A	374	ARG	Sidechain
1	A	88	ARG	Sidechain

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	3081	0	3011	409	1
2	A	5	0	0	0	0
All	All	3086	0	3011	409	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 67.

All (409) 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:258:LLP:C4'	1:A:258:LLP:NZ	1.85	1.39
1:A:252:VAL:HG13	1:A:271:THR:HG23	1.26	1.14
1:A:112:THR:HG21	1:A:118:ALA:HB2	1.27	1.09
1:A:231:ARG:HG2	1:A:357:ASN:HD22	1.10	1.09
1:A:193:CYS:SG	1:A:200:ASP:HB3	1.94	1.07
1:A:28:LEU:HB2	1:A:382:VAL:HG13	1.35	1.06
1:A:333:MET:HE1	1:A:336:LEU:HD23	1.41	1.01
1:A:230:ALA:HB3	1:A:358:GLY:H	1.26	0.99
1:A:218:TRP:O	1:A:219:LEU:HB2	1.65	0.95
1:A:333:MET:HE3	1:A:333:MET:HA	1.48	0.94
1:A:83:ILE:HG22	1:A:84:PRO:HD2	1.46	0.94
1:A:345:GLY:HA2	1:A:405:VAL:HG11	1.48	0.94
1:A:112:THR:HG21	1:A:118:ALA:CB	1.97	0.94
1:A:146:LYS:HG2	1:A:156:VAL:HG21	1.50	0.92
1:A:223:ASP:OD2	1:A:258:LLP:N1	2.02	0.92
1:A:231:ARG:HG2	1:A:357:ASN:ND2	1.86	0.90
1:A:112:THR:CG2	1:A:118:ALA:HB2	2.01	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:ARG:CG	1:A:357:ASN:HD22	1.85	0.89
1:A:134:ARG:HH11	1:A:157:ARG:HG2	1.37	0.89
1:A:195:ASN:OD1	1:A:196:PRO:HA	1.72	0.88
1:A:370:VAL:HG11	1:A:383:ALA:HA	1.55	0.87
1:A:231:ARG:HG3	1:A:231:ARG:HH11	1.38	0.86
1:A:194:HIS:HB3	1:A:197:THR:O	1.76	0.86
1:A:337:PHE:CD2	1:A:392:MET:HE1	2.14	0.83
1:A:140:PRO:HB2	1:A:196:PRO:HD2	1.60	0.83
1:A:397:MET:HE2	1:A:401:CYS:SG	2.20	0.81
1:A:220:PRO:HD3	1:A:247:HIS:CE1	2.15	0.81
1:A:238:GLU:HB2	1:A:241:ARG:HD3	1.61	0.81
1:A:137:VAL:HG21	1:A:156:VAL:HB	1.62	0.81
1:A:137:VAL:HG11	1:A:158:GLU:HG2	1.62	0.81
1:A:208:THR:HG22	1:A:209:LEU:HD13	1.63	0.81
1:A:399:PRO:O	1:A:402:GLU:HG3	1.83	0.79
1:A:300:ALA:O	1:A:303:ALA:HB3	1.83	0.78
1:A:142:TRP:O	1:A:145:HIS:HB2	1.84	0.78
1:A:324:THR:HA	1:A:327:ARG:HD3	1.64	0.78
1:A:108:ARG:HB2	1:A:280:VAL:HG23	1.64	0.77
1:A:333:MET:HG3	1:A:392:MET:HB3	1.66	0.77
1:A:292:ASP:HA	1:A:296:SER:HA	1.68	0.76
1:A:203:LEU:HD13	1:A:207:GLN:HG3	1.68	0.76
1:A:87:GLY:O	1:A:91:GLN:HB2	1.87	0.75
1:A:393:THR:HB	1:A:396:ASN:HB2	1.69	0.75
1:A:371:LEU:C	1:A:373:LEU:H	1.92	0.75
1:A:116:THR:HB	1:A:258:LLP:OP2	1.85	0.74
1:A:85:GLU:HG3	1:A:88:ARG:HH21	1.52	0.74
1:A:67:TYR:O	1:A:71:ASN:HB2	1.87	0.74
1:A:47:VAL:HG22	1:A:263:TYR:CE1	2.23	0.74
1:A:79:GLY:O	1:A:298:PRO:HD2	1.88	0.73
1:A:174:LEU:O	1:A:178:LEU:HB3	1.87	0.72
1:A:169:LEU:HB2	1:A:199:ILE:CG2	2.19	0.72
1:A:160:ALA:O	1:A:174:LEU:HB2	1.89	0.72
1:A:333:MET:CE	1:A:336:LEU:HD23	2.18	0.72
1:A:231:ARG:HB2	1:A:236:ASP:HB2	1.72	0.71
1:A:252:VAL:HG13	1:A:271:THR:CG2	2.14	0.71
1:A:373:LEU:HD13	1:A:407:VAL:HG11	1.72	0.71
1:A:134:ARG:HD2	1:A:157:ARG:HG2	1.72	0.71
1:A:82:GLY:CA	1:A:298:PRO:HG3	2.20	0.71
1:A:213:SER:HG	1:A:218:TRP:HE3	1.39	0.70
1:A:46:GLY:HA2	1:A:360:PHE:HZ	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HG22	1:A:258:LLP:OP2	1.90	0.70
1:A:373:LEU:HG	1:A:379:VAL:HG13	1.73	0.70
1:A:111:GLN:HE21	1:A:298:PRO:HB2	1.54	0.70
1:A:146:LYS:HG2	1:A:156:VAL:CG2	2.22	0.70
1:A:193:CYS:HG	1:A:200:ASP:HB3	1.57	0.70
1:A:252:VAL:CG1	1:A:271:THR:HG23	2.15	0.69
1:A:40:LYS:HE2	1:A:400:LEU:HD13	1.74	0.69
1:A:359:MET:HG3	1:A:388:ASN:OD1	1.93	0.69
1:A:128:LYS:HD2	1:A:129:ASN:N	2.07	0.69
1:A:80:ILE:HD12	1:A:297:ASN:H	1.57	0.69
1:A:171:PHE:HA	1:A:174:LEU:HD23	1.75	0.69
1:A:348:ARG:HH22	1:A:365:LEU:CD2	2.05	0.69
1:A:397:MET:HE3	1:A:400:LEU:HD23	1.74	0.69
1:A:110:ALA:O	1:A:269:ALA:HA	1.92	0.68
1:A:116:THR:CB	1:A:258:LLP:OP2	2.40	0.68
1:A:208:THR:HA	1:A:211:GLN:NE2	2.08	0.68
1:A:369:GLN:O	1:A:373:LEU:HB2	1.94	0.68
1:A:243:PHE:O	1:A:246:MET:HB2	1.93	0.68
1:A:28:LEU:HG	1:A:380:TYR:HD2	1.57	0.68
1:A:377:PHE:HB3	1:A:379:VAL:HG12	1.75	0.68
1:A:134:ARG:HG3	1:A:135:VAL:N	2.09	0.67
1:A:309:ILE:HG23	1:A:316:ARG:CA	2.24	0.67
1:A:345:GLY:HA2	1:A:405:VAL:CG1	2.22	0.67
1:A:136:TRP:HE3	1:A:159:TYR:HD2	1.40	0.67
1:A:193:CYS:SG	1:A:357:ASN:HB3	2.34	0.67
1:A:231:ARG:HG3	1:A:231:ARG:NH1	2.04	0.66
1:A:40:LYS:HZ3	1:A:43:LEU:HD22	1.60	0.66
1:A:365:LEU:HD13	1:A:369:GLN:HB3	1.78	0.66
1:A:334:ARG:O	1:A:338:VAL:HG23	1.96	0.65
1:A:135:VAL:O	1:A:156:VAL:HA	1.96	0.65
1:A:146:LYS:HA	1:A:156:VAL:HG21	1.79	0.65
1:A:393:THR:O	1:A:397:MET:N	2.30	0.65
1:A:128:LYS:NZ	1:A:129:ASN:HB2	2.11	0.65
1:A:294:ASN:HD22	1:A:295:TYR:HD1	1.44	0.65
1:A:116:THR:CG2	1:A:258:LLP:OP2	2.44	0.64
1:A:134:ARG:HD2	1:A:157:ARG:CG	2.27	0.64
1:A:348:ARG:HH22	1:A:365:LEU:HD23	1.59	0.64
1:A:309:ILE:HG23	1:A:316:ARG:HA	1.78	0.64
1:A:393:THR:HG23	1:A:394:PRO:HD2	1.80	0.64
1:A:86:PHE:O	1:A:90:THR:HB	1.98	0.64
1:A:333:MET:HG3	1:A:392:MET:CB	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LEU:HD21	1:A:380:TYR:HB3	1.80	0.64
1:A:35:ASP:HB2	1:A:37:ARG:HH21	1.63	0.63
1:A:142:TRP:CZ2	1:A:144:ASN:HB3	2.34	0.63
1:A:96:GLY:HA3	1:A:102:ILE:HD11	1.81	0.63
1:A:40:LYS:NZ	1:A:43:LEU:HD22	2.14	0.63
1:A:31:LEU:HD12	1:A:31:LEU:H	1.63	0.62
1:A:91:GLN:HA	1:A:94:LEU:HD12	1.82	0.62
1:A:334:ARG:CG	1:A:353:ILE:HG12	2.29	0.62
1:A:339:ASN:C	1:A:341:LEU:H	2.07	0.62
1:A:122:ALA:O	1:A:126:LEU:HB3	2.00	0.62
1:A:13:MET:HG3	1:A:14:PHE:N	2.12	0.62
1:A:40:LYS:O	1:A:41:ILE:HG13	1.99	0.62
1:A:247:HIS:O	1:A:248:LYS:HG3	1.99	0.62
1:A:330:ILE:HG21	1:A:358:GLY:O	2.00	0.62
1:A:359:MET:SD	1:A:390:ALA:HB2	2.39	0.62
1:A:83:ILE:CG2	1:A:84:PRO:HD2	2.26	0.62
1:A:20:ALA:HB3	1:A:21:PRO:HD3	1.82	0.61
1:A:140:PRO:HB2	1:A:196:PRO:CD	2.29	0.61
1:A:137:VAL:CG2	1:A:156:VAL:HB	2.29	0.61
1:A:48:TYR:OH	1:A:329:ARG:HB3	1.99	0.61
1:A:189:PHE:O	1:A:222:PHE:HA	2.00	0.61
1:A:221:LEU:HD12	1:A:222:PHE:N	2.16	0.61
1:A:159:TYR:HB3	1:A:178:LEU:HA	1.83	0.61
1:A:40:LYS:CE	1:A:400:LEU:HD13	2.31	0.60
1:A:334:ARG:HG2	1:A:353:ILE:HG12	1.83	0.60
1:A:188:LEU:HB2	1:A:221:LEU:HG	1.82	0.60
1:A:371:LEU:C	1:A:373:LEU:N	2.60	0.60
1:A:41:ILE:HG23	1:A:42:ASN:H	1.65	0.60
1:A:155:GLU:HA	1:A:155:GLU:OE1	2.01	0.60
1:A:99:SER:O	1:A:102:ILE:HB	2.02	0.60
1:A:284:PHE:HA	1:A:287:MET:HB3	1.82	0.60
1:A:353:ILE:HG23	1:A:354:ILE:H	1.65	0.60
1:A:276:ASP:HB3	1:A:279:THR:OG1	2.02	0.59
1:A:13:MET:HG3	1:A:14:PHE:HB3	1.84	0.59
1:A:41:ILE:CG2	1:A:42:ASN:N	2.65	0.59
1:A:248:LYS:HB3	1:A:275:ALA:HB2	1.85	0.59
1:A:323:LEU:O	1:A:327:ARG:HG3	2.02	0.59
1:A:89:CYS:HA	1:A:92:GLU:HG2	1.84	0.59
1:A:82:GLY:HA2	1:A:298:PRO:HG3	1.85	0.59
1:A:64:ALA:O	1:A:67:TYR:HB3	2.03	0.59
1:A:231:ARG:HB2	1:A:236:ASP:CB	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:O	1:A:340:THR:OG1	2.20	0.59
1:A:402:GLU:OE2	1:A:403:ALA:HB2	2.03	0.58
1:A:95:PHE:HD2	1:A:240:LEU:HD21	1.66	0.58
1:A:114:GLY:C	1:A:116:THR:H	2.11	0.58
1:A:238:GLU:HA	1:A:241:ARG:CB	2.34	0.58
1:A:386:ARG:C	1:A:386:ARG:HH11	2.12	0.58
1:A:91:GLN:HE22	1:A:107:ALA:HB3	1.69	0.58
1:A:170:ASP:O	1:A:174:LEU:HB3	2.04	0.57
1:A:368:GLU:HA	1:A:371:LEU:HB3	1.85	0.57
1:A:47:VAL:HG22	1:A:263:TYR:CD1	2.40	0.57
1:A:286:GLN:O	1:A:289:ALA:HB3	2.03	0.57
1:A:353:ILE:HG23	1:A:354:ILE:HD12	1.85	0.57
1:A:61:VAL:HG12	1:A:62:LYS:N	2.19	0.57
1:A:134:ARG:HD2	1:A:157:ARG:HB2	1.85	0.57
1:A:208:THR:HA	1:A:211:GLN:HE22	1.68	0.57
1:A:169:LEU:HB2	1:A:199:ILE:HG21	1.86	0.57
1:A:333:MET:HA	1:A:333:MET:CE	2.30	0.56
1:A:398:ALA:N	1:A:399:PRO:HD2	2.20	0.56
1:A:58:LEU:HB2	1:A:61:VAL:HG21	1.87	0.56
1:A:309:ILE:HG23	1:A:316:ARG:HB3	1.87	0.56
1:A:46:GLY:HA2	1:A:360:PHE:CZ	2.40	0.56
1:A:180:GLU:HG2	1:A:181:ALA:N	2.20	0.56
1:A:231:ARG:CB	1:A:357:ASN:HD22	2.19	0.56
1:A:339:ASN:O	1:A:341:LEU:N	2.39	0.56
1:A:112:THR:CB	1:A:118:ALA:HB2	2.36	0.55
1:A:288:LYS:CE	1:A:288:LYS:HA	2.37	0.55
1:A:196:PRO:HB2	1:A:386:ARG:HG3	1.88	0.55
1:A:128:LYS:HZ3	1:A:286:GLN:HB3	1.71	0.55
1:A:203:LEU:HD13	1:A:207:GLN:CG	2.36	0.55
1:A:288:LYS:HA	1:A:288:LYS:NZ	2.21	0.55
1:A:325:ASP:O	1:A:329:ARG:HB2	2.06	0.55
1:A:41:ILE:CG2	1:A:42:ASN:H	2.20	0.55
1:A:386:ARG:HB3	1:A:386:ARG:CZ	2.36	0.55
1:A:100:ALA:O	1:A:104:ASP:N	2.40	0.54
1:A:180:GLU:HG2	1:A:181:ALA:H	1.71	0.54
1:A:188:LEU:HA	1:A:221:LEU:O	2.06	0.54
1:A:367:LYS:HD3	1:A:367:LYS:N	2.22	0.54
1:A:167:HIS:O	1:A:199:ILE:HD11	2.08	0.54
1:A:111:GLN:OE1	1:A:267:VAL:HG23	2.07	0.54
1:A:228:GLY:O	1:A:327:ARG:HD2	2.08	0.54
1:A:260:PHE:HE1	1:A:309:ILE:HD13	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:LEU:HD12	1:A:31:LEU:N	2.20	0.54
1:A:386:ARG:HB3	1:A:386:ARG:NH1	2.22	0.54
1:A:230:ALA:HB3	1:A:358:GLY:N	2.09	0.54
1:A:91:GLN:HE22	1:A:107:ALA:CB	2.21	0.54
1:A:282:ARG:HG3	1:A:282:ARG:HH11	1.73	0.54
1:A:163:ASP:HB2	1:A:170:ASP:HB2	1.90	0.54
1:A:404:ILE:O	1:A:408:LEU:OXT	2.25	0.54
1:A:124:ASP:OD1	1:A:152:ALA:HB3	2.08	0.53
1:A:137:VAL:CG1	1:A:158:GLU:HG2	2.33	0.53
1:A:153:GLY:O	1:A:154:LEU:O	2.26	0.53
1:A:229:PHE:HA	1:A:327:ARG:HG2	1.90	0.53
1:A:365:LEU:HD22	1:A:369:GLN:CD	2.33	0.53
1:A:64:ALA:O	1:A:68:LEU:HD13	2.08	0.53
1:A:294:ASN:ND2	1:A:295:TYR:HD1	2.06	0.53
1:A:80:ILE:HD12	1:A:297:ASN:N	2.24	0.53
1:A:137:VAL:HG12	1:A:158:GLU:HA	1.91	0.53
1:A:40:LYS:HG3	1:A:399:PRO:HG2	1.91	0.53
1:A:202:THR:H	1:A:205:GLN:HE21	1.56	0.53
1:A:230:ALA:CB	1:A:358:GLY:H	2.11	0.53
1:A:341:LEU:HB3	1:A:350:PHE:CD2	2.44	0.53
1:A:135:VAL:HG13	1:A:156:VAL:HG12	1.91	0.53
1:A:82:GLY:HA3	1:A:111:GLN:CB	2.39	0.52
1:A:256:TYR:O	1:A:260:PHE:HB2	2.08	0.52
1:A:197:THR:HG21	1:A:199:ILE:HD12	1.91	0.52
1:A:42:ASN:OD1	1:A:45:ILE:HG21	2.09	0.52
1:A:338:VAL:HG21	1:A:353:ILE:CG2	2.39	0.52
1:A:339:ASN:O	1:A:343:GLU:N	2.36	0.52
1:A:28:LEU:HD21	1:A:380:TYR:C	2.35	0.52
1:A:41:ILE:HG22	1:A:43:LEU:H	1.74	0.52
1:A:145:HIS:O	1:A:149:PHE:CD2	2.62	0.52
1:A:401:CYS:O	1:A:405:VAL:HG22	2.10	0.52
1:A:96:GLY:HA3	1:A:102:ILE:CD1	2.39	0.52
1:A:220:PRO:HD3	1:A:247:HIS:NE2	2.25	0.52
1:A:60:SER:OG	1:A:319:TRP:HB2	2.10	0.51
1:A:162:TYR:CD1	1:A:197:THR:HG21	2.45	0.51
1:A:163:ASP:CG	1:A:170:ASP:HB2	2.36	0.51
1:A:397:MET:CE	1:A:400:LEU:HD23	2.40	0.51
1:A:26:LEU:C	1:A:28:LEU:N	2.64	0.51
1:A:309:ILE:HG22	1:A:310:LEU:HD13	1.91	0.51
1:A:136:TRP:CE3	1:A:159:TYR:HD2	2.26	0.51
1:A:179:ASN:HA	1:A:218:TRP:HZ2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:NZ	1:A:286:GLN:HB3	2.26	0.51
1:A:167:HIS:CD2	1:A:167:HIS:H	2.22	0.51
1:A:187:VAL:O	1:A:221:LEU:HB3	2.11	0.51
1:A:135:VAL:HG13	1:A:156:VAL:CG1	2.41	0.51
1:A:24:PRO:C	1:A:26:LEU:N	2.67	0.51
1:A:188:LEU:HD12	1:A:221:LEU:HD12	1.92	0.51
1:A:349:ASP:O	1:A:352:PHE:HE1	1.93	0.51
1:A:80:ILE:HD11	1:A:292:ASP:N	2.26	0.50
1:A:227:GLN:HE21	1:A:237:ALA:HB2	1.76	0.50
1:A:171:PHE:HA	1:A:174:LEU:CD2	2.41	0.50
1:A:203:LEU:HD21	1:A:242:ALA:HB2	1.92	0.50
1:A:238:GLU:HA	1:A:241:ARG:HB3	1.93	0.50
1:A:330:ILE:HG21	1:A:359:MET:HA	1.93	0.50
1:A:340:THR:O	1:A:344:LYS:CB	2.60	0.50
1:A:341:LEU:O	1:A:344:LYS:C	2.54	0.50
1:A:140:PRO:CB	1:A:196:PRO:HD2	2.38	0.50
1:A:42:ASN:H	1:A:42:ASN:ND2	2.10	0.50
1:A:363:SER:N	1:A:385:GLY:O	2.45	0.50
1:A:128:LYS:HZ3	1:A:129:ASN:HB2	1.75	0.50
1:A:142:TRP:CE2	1:A:144:ASN:HB3	2.47	0.50
1:A:233:LEU:CD1	1:A:323:LEU:HD21	2.42	0.50
1:A:84:PRO:HG2	1:A:85:GLU:OE2	2.12	0.50
1:A:312:ASN:HB3	1:A:315:LEU:HB2	1.93	0.49
1:A:40:LYS:HG2	1:A:396:ASN:CG	2.36	0.49
1:A:309:ILE:CG2	1:A:316:ARG:HB3	2.42	0.49
1:A:238:GLU:HA	1:A:241:ARG:HB2	1.95	0.49
1:A:309:ILE:HG13	1:A:315:LEU:HG	1.94	0.49
1:A:294:ASN:ND2	1:A:295:TYR:CD1	2.81	0.49
1:A:229:PHE:HD1	1:A:330:ILE:HD11	1.77	0.49
1:A:295:TYR:O	1:A:295:TYR:CG	2.65	0.49
1:A:106:ARG:HG3	1:A:275:ALA:HA	1.94	0.48
1:A:312:ASN:HB3	1:A:315:LEU:CB	2.43	0.48
1:A:48:TYR:HH	1:A:329:ARG:HB3	1.76	0.48
1:A:188:LEU:HD12	1:A:221:LEU:CD1	2.44	0.48
1:A:194:HIS:HB2	1:A:199:ILE:O	2.13	0.48
1:A:219:LEU:HA	1:A:247:HIS:CE1	2.48	0.48
1:A:309:ILE:HG22	1:A:310:LEU:N	2.27	0.48
1:A:230:ALA:HB3	1:A:357:ASN:HA	1.95	0.48
1:A:372:ARG:NH2	1:A:407:VAL:HA	2.28	0.48
1:A:309:ILE:HG23	1:A:316:ARG:CB	2.43	0.48
1:A:75:LYS:HB2	1:A:75:LYS:HE2	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:THR:O	1:A:344:LYS:HB2	2.13	0.48
1:A:389:VAL:HA	1:A:392:MET:HG3	1.95	0.48
1:A:28:LEU:CD2	1:A:380:TYR:HB3	2.44	0.48
1:A:136:TRP:HB2	1:A:186:VAL:O	2.14	0.48
1:A:291:ILE:HG23	1:A:295:TYR:CZ	2.48	0.48
1:A:274:ALA:HB3	1:A:280:VAL:HA	1.96	0.47
1:A:339:ASN:C	1:A:341:LEU:N	2.67	0.47
1:A:354:ILE:H	1:A:354:ILE:HD12	1.79	0.47
1:A:397:MET:HE3	1:A:397:MET:HA	1.95	0.47
1:A:47:VAL:HG22	1:A:263:TYR:CZ	2.48	0.47
1:A:159:TYR:CG	1:A:178:LEU:HB2	2.49	0.47
1:A:256:TYR:HA	1:A:259:ASN:OD1	2.13	0.47
1:A:339:ASN:OD1	1:A:343:GLU:HB2	2.13	0.47
1:A:58:LEU:HB2	1:A:61:VAL:CG2	2.44	0.47
1:A:40:LYS:HB3	1:A:40:LYS:HE3	1.56	0.47
1:A:284:PHE:CE2	1:A:287:MET:HG2	2.50	0.47
1:A:17:ILE:HG23	1:A:17:ILE:O	2.15	0.47
1:A:128:LYS:C	1:A:130:THR:H	2.22	0.47
1:A:185:ASP:O	1:A:218:TRP:HA	2.15	0.47
1:A:277:SER:N	1:A:280:VAL:HG13	2.29	0.47
1:A:20:ALA:HB3	1:A:21:PRO:CD	2.45	0.47
1:A:272:LEU:HB2	1:A:287:MET:CE	2.44	0.47
1:A:324:THR:CA	1:A:327:ARG:HD3	2.41	0.47
1:A:51:GLU:HG3	1:A:329:ARG:HE	1.80	0.46
1:A:82:GLY:HA3	1:A:111:GLN:HB2	1.98	0.46
1:A:377:PHE:O	1:A:378:GLY:C	2.58	0.46
1:A:189:PHE:HB2	1:A:222:PHE:CD2	2.51	0.46
1:A:228:GLY:N	1:A:233:LEU:HA	2.30	0.46
1:A:238:GLU:CB	1:A:241:ARG:HD3	2.39	0.46
1:A:321:GLN:HA	1:A:324:THR:OG1	2.16	0.46
1:A:43:LEU:HD23	1:A:380:TYR:O	2.16	0.46
1:A:224:PHE:HB3	1:A:254:SER:OG	2.14	0.46
1:A:353:ILE:HG23	1:A:354:ILE:CD1	2.45	0.46
1:A:191:GLY:HA2	1:A:222:PHE:HE1	1.81	0.46
1:A:301:HIS:O	1:A:304:SER:HB2	2.16	0.46
1:A:28:LEU:CG	1:A:29:ALA:H	2.26	0.46
1:A:62:LYS:HD3	1:A:62:LYS:HA	1.58	0.46
1:A:351:SER:O	1:A:354:ILE:HD12	2.15	0.46
1:A:196:PRO:CB	1:A:386:ARG:HG3	2.45	0.46
1:A:202:THR:H	1:A:205:GLN:HB2	1.80	0.46
1:A:20:ALA:H	1:A:21:PRO:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ILE:HA	1:A:297:ASN:HA	1.97	0.46
1:A:112:THR:O	1:A:112:THR:HG22	2.16	0.46
1:A:128:LYS:O	1:A:129:ASN:HB3	2.14	0.46
1:A:134:ARG:HD2	1:A:157:ARG:CB	2.44	0.46
1:A:162:TYR:HD1	1:A:199:ILE:CD1	2.29	0.46
1:A:150:ASN:HA	1:A:153:GLY:O	2.16	0.46
1:A:201:PRO:HA	1:A:205:GLN:NE2	2.31	0.46
1:A:142:TRP:HE3	1:A:145:HIS:CE1	2.33	0.46
1:A:371:LEU:HD12	1:A:374:ARG:HD2	1.97	0.46
1:A:64:ALA:HB1	1:A:308:THR:HG21	1.98	0.45
1:A:196:PRO:HB2	1:A:362:PHE:CE1	2.51	0.45
1:A:106:ARG:HA	1:A:280:VAL:HG11	1.97	0.45
1:A:145:HIS:O	1:A:149:PHE:HD2	2.00	0.45
1:A:341:LEU:HA	1:A:345:GLY:N	2.31	0.45
1:A:35:ASP:HB2	1:A:37:ARG:NH2	2.29	0.45
1:A:112:THR:HG21	1:A:118:ALA:CA	2.44	0.45
1:A:85:GLU:HG3	1:A:88:ARG:NH2	2.26	0.45
1:A:82:GLY:HA2	1:A:298:PRO:CG	2.46	0.45
1:A:134:ARG:NH1	1:A:157:ARG:HG2	2.18	0.45
1:A:196:PRO:HB2	1:A:362:PHE:CD1	2.52	0.45
1:A:210:ALA:HB1	1:A:246:MET:SD	2.57	0.45
1:A:231:ARG:CG	1:A:357:ASN:ND2	2.63	0.44
1:A:348:ARG:HH22	1:A:365:LEU:HD21	1.79	0.44
1:A:121:VAL:O	1:A:125:PHE:HB3	2.17	0.44
1:A:242:ALA:O	1:A:246:MET:HG3	2.17	0.44
1:A:333:MET:HB3	1:A:389:VAL:CG1	2.47	0.44
1:A:333:MET:HB3	1:A:389:VAL:HG13	1.99	0.44
1:A:43:LEU:HA	1:A:45:ILE:CD1	2.48	0.44
1:A:87:GLY:O	1:A:91:GLN:CB	2.63	0.44
1:A:203:LEU:O	1:A:207:GLN:HG3	2.17	0.44
1:A:338:VAL:CG2	1:A:353:ILE:HG21	2.48	0.44
1:A:136:TRP:CE3	1:A:157:ARG:O	2.70	0.44
1:A:180:GLU:CG	1:A:181:ALA:N	2.76	0.44
1:A:95:PHE:CD2	1:A:240:LEU:HD21	2.51	0.44
1:A:135:VAL:O	1:A:157:ARG:N	2.51	0.44
1:A:171:PHE:O	1:A:175:ILE:HB	2.18	0.44
1:A:186:VAL:HG12	1:A:219:LEU:O	2.18	0.44
1:A:282:ARG:C	1:A:284:PHE:N	2.70	0.44
1:A:316:ARG:HA	1:A:319:TRP:HB3	1.98	0.44
1:A:334:ARG:HB3	1:A:354:ILE:HG13	2.00	0.44
1:A:135:VAL:HG13	1:A:156:VAL:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:LEU:HA	1:A:212:LEU:HB2	2.00	0.44
1:A:201:PRO:HA	1:A:205:GLN:HE21	1.83	0.43
1:A:284:PHE:C	1:A:286:GLN:N	2.72	0.43
1:A:260:PHE:CE1	1:A:309:ILE:HD13	2.52	0.43
1:A:328:GLN:O	1:A:332:ARG:HB2	2.18	0.43
1:A:316:ARG:H	1:A:316:ARG:HG3	1.58	0.43
1:A:284:PHE:C	1:A:287:MET:H	2.27	0.43
1:A:373:LEU:HD12	1:A:373:LEU:HA	1.82	0.43
1:A:274:ALA:HB3	1:A:280:VAL:CA	2.49	0.43
1:A:365:LEU:HD22	1:A:369:GLN:NE2	2.33	0.43
1:A:112:THR:O	1:A:114:GLY:N	2.50	0.43
1:A:260:PHE:CD2	1:A:306:VAL:HG22	2.52	0.43
1:A:31:LEU:O	1:A:34:ALA:HB2	2.19	0.43
1:A:83:ILE:H	1:A:83:ILE:HG12	1.76	0.42
1:A:28:LEU:HG	1:A:29:ALA:H	1.84	0.42
1:A:68:LEU:O	1:A:72:GLU:HB2	2.20	0.42
1:A:114:GLY:C	1:A:116:THR:N	2.77	0.42
1:A:203:LEU:O	1:A:207:GLN:HB2	2.18	0.42
1:A:288:LYS:HA	1:A:288:LYS:HE3	2.01	0.42
1:A:168:THR:HA	1:A:199:ILE:CD1	2.50	0.42
1:A:228:GLY:HA3	1:A:233:LEU:HB2	2.01	0.42
1:A:86:PHE:CE1	1:A:256:TYR:HE2	2.37	0.42
1:A:138:SER:O	1:A:141:SER:HB3	2.19	0.42
1:A:250:LEU:O	1:A:251:ILE:HG22	2.19	0.42
1:A:353:ILE:HA	1:A:356:GLN:OE1	2.19	0.42
1:A:206:TRP:CH2	1:A:222:PHE:CZ	3.08	0.42
1:A:272:LEU:HD21	1:A:274:ALA:HB2	2.02	0.42
1:A:369:GLN:HE21	1:A:407:VAL:HG23	1.84	0.42
1:A:85:GLU:C	1:A:87:GLY:N	2.74	0.42
1:A:90:THR:CG2	1:A:91:GLN:N	2.82	0.42
1:A:359:MET:SD	1:A:390:ALA:CB	3.08	0.42
1:A:81:ASP:OD2	1:A:288:LYS:HE2	2.20	0.42
1:A:163:ASP:CB	1:A:170:ASP:HB2	2.50	0.42
1:A:140:PRO:CB	1:A:196:PRO:CD	2.98	0.41
1:A:213:SER:OG	1:A:218:TRP:HE3	2.00	0.41
1:A:277:SER:CA	1:A:280:VAL:HG13	2.49	0.41
1:A:327:ARG:O	1:A:330:ILE:N	2.53	0.41
1:A:334:ARG:HB3	1:A:354:ILE:HA	2.01	0.41
1:A:26:LEU:C	1:A:28:LEU:H	2.24	0.41
1:A:89:CYS:HA	1:A:92:GLU:CG	2.50	0.41
1:A:284:PHE:O	1:A:288:LYS:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LEU:HA	1:A:341:LEU:HD23	1.85	0.41
1:A:344:LYS:HD2	1:A:344:LYS:HA	1.88	0.41
1:A:37:ARG:HA	1:A:37:ARG:HD3	1.97	0.41
1:A:146:LYS:O	1:A:150:ASN:OD1	2.37	0.41
1:A:227:GLN:NE2	1:A:237:ALA:HB2	2.34	0.41
1:A:258:LLP:C4'	1:A:258:LLP:OP4	2.68	0.41
1:A:345:GLY:O	1:A:346:ALA:C	2.63	0.41
1:A:282:ARG:C	1:A:284:PHE:H	2.28	0.41
1:A:44:GLY:H	1:A:45:ILE:HG12	1.85	0.41
1:A:188:LEU:HD11	1:A:223:ASP:HB2	2.02	0.41
1:A:41:ILE:HG23	1:A:42:ASN:CG	2.46	0.41
1:A:193:CYS:HB3	1:A:198:GLY:O	2.20	0.41
1:A:393:THR:HG23	1:A:394:PRO:CD	2.49	0.41
1:A:397:MET:O	1:A:400:LEU:HB3	2.21	0.41
1:A:67:TYR:CD1	1:A:67:TYR:C	2.99	0.41
1:A:139:ASN:HA	1:A:140:PRO:C	2.44	0.41
1:A:25:ILE:HG22	1:A:26:LEU:N	2.32	0.40
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.86	0.40
1:A:44:GLY:H	1:A:388:ASN:HB2	1.86	0.40
1:A:235:GLU:O	1:A:235:GLU:HG2	2.21	0.40
1:A:170:ASP:HB3	1:A:173:ALA:HB3	2.02	0.40
1:A:309:ILE:CG2	1:A:316:ARG:HA	2.49	0.40
1:A:40:LYS:HE3	1:A:41:ILE:H	1.86	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)
1:A:144:ASN:ND2	1:A:292:ASP:OD1[4_566]	2.11	0.09

5.3 Torsion angles

5.3.1 Protein backbone

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	393/396 (99%)	273 (70%)	73 (19%)	47 (12%)	0 1

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	21	PRO
1	A	29	ALA
1	A	39	GLY
1	A	43	LEU
1	A	58	LEU
1	A	59	THR
1	A	97	LYS
1	A	138	SER
1	A	154	LEU
1	A	158	GLU
1	A	165	GLU
1	A	167	HIS
1	A	180	GLU
1	A	183	ALA
1	A	219	LEU
1	A	247	HIS
1	A	248	LYS
1	A	277	SER
1	A	301	HIS
1	A	345	GLY
1	A	352	PHE
1	A	367	LYS
1	A	377	PHE
1	A	383	ALA
1	A	393	THR
1	A	46	GLY
1	A	96	GLY
1	A	182	GLN
1	A	191	GLY
1	A	233	LEU
1	A	240	LEU
1	A	340	THR
1	A	20	ALA
1	A	266	ARG
1	A	275	ALA
1	A	346	ALA
1	A	351	SER

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Mol	Chain	Res	Type
1	A	366	THR
1	A	401	CYS
1	A	40	LYS
1	A	382	VAL
1	A	297	ASN
1	A	24	PRO
1	A	17	ILE
1	A	354	ILE
1	A	378	GLY

5.3.2 Protein sidechains ⓘ

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	319/319 (100%)	191 (60%)	128 (40%)	0 0

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	15	GLU
1	A	16	ASN
1	A	17	ILE
1	A	18	THR
1	A	21	PRO
1	A	25	ILE
1	A	31	LEU
1	A	33	ARG
1	A	36	GLU
1	A	37	ARG
1	A	38	PRO
1	A	40	LYS
1	A	42	ASN
1	A	45	ILE
1	A	47	VAL
1	A	51	GLU

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Mol	Chain	Res	Type
1	A	52	THR
1	A	57	VAL
1	A	58	LEU
1	A	61	VAL
1	A	69	LEU
1	A	71	ASN
1	A	73	THR
1	A	75	LYS
1	A	78	LEU
1	A	81	ASP
1	A	83	ILE
1	A	88	ARG
1	A	90	THR
1	A	93	LEU
1	A	95	PHE
1	A	99	SER
1	A	101	LEU
1	A	102	ILE
1	A	108	ARG
1	A	109	THR
1	A	112	THR
1	A	116	THR
1	A	121	VAL
1	A	124	ASP
1	A	125	PHE
1	A	126	LEU
1	A	128	LYS
1	A	135	VAL
1	A	137	VAL
1	A	146	LYS
1	A	147	SER
1	A	150	ASN
1	A	151	SER
1	A	154	LEU
1	A	155	GLU
1	A	157	ARG
1	A	169	LEU
1	A	172	ASP
1	A	174	LEU
1	A	175	ILE
1	A	178	LEU
1	A	188	LEU

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Mol	Chain	Res	Type
1	A	190	HIS
1	A	194	HIS
1	A	197	THR
1	A	203	LEU
1	A	208	THR
1	A	209	LEU
1	A	211	GLN
1	A	214	VAL
1	A	215	GLU
1	A	216	LYS
1	A	219	LEU
1	A	221	LEU
1	A	222	PHE
1	A	224	PHE
1	A	231	ARG
1	A	234	GLU
1	A	235	GLU
1	A	236	ASP
1	A	238	GLU
1	A	240	LEU
1	A	247	HIS
1	A	251	ILE
1	A	254	SER
1	A	260	PHE
1	A	262	LEU
1	A	264	ASN
1	A	265	GLU
1	A	266	ARG
1	A	270	CYS
1	A	271	THR
1	A	273	VAL
1	A	279	THR
1	A	280	VAL
1	A	281	ASP
1	A	287	MET
1	A	288	LYS
1	A	294	ASN
1	A	297	ASN
1	A	308	THR
1	A	309	ILE
1	A	310	LEU
1	A	311	SER

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Mol	Chain	Res	Type
1	A	313	ASP
1	A	316	ARG
1	A	320	GLU
1	A	321	GLN
1	A	328	GLN
1	A	329	ARG
1	A	332	ARG
1	A	333	MET
1	A	334	ARG
1	A	339	ASN
1	A	340	THR
1	A	344	LYS
1	A	363	SER
1	A	365	LEU
1	A	366	THR
1	A	368	GLU
1	A	370	VAL
1	A	374	ARG
1	A	375	GLU
1	A	376	GLU
1	A	379	VAL
1	A	382	VAL
1	A	384	SER
1	A	386	ARG
1	A	392	MET
1	A	405	VAL
1	A	408	LEU

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

Mol	Chain	Res	Type
1	A	16	ASN
1	A	76	ASN
1	A	91	GLN
1	A	129	ASN
1	A	144	ASN
1	A	167	HIS
1	A	194	HIS
1	A	205	GLN
1	A	227	GLN
1	A	247	HIS
1	A	294	ASN

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Mol	Chain	Res	Type
1	A	328	GLN
1	A	331	GLN
1	A	357	ASN
1	A	369	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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$
1	LLP	A	258	1	23,24,25	4.01	4 (17%)	25,32,34	3.93	12 (48%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	258	1	-	13/16/17/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	LLP	C4'-NZ	17.32	1.85	1.27
1	A	258	LLP	O3-C3	-6.58	1.21	1.36
1	A	258	LLP	C4-C5	-3.20	1.37	1.42
1	A	258	LLP	C3-C2	2.33	1.43	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	LLP	CE-NZ-C4'	12.02	157.21	118.72
1	A	258	LLP	C4-C3-C2	-8.65	115.28	120.14
1	A	258	LLP	C3-C4-C5	6.79	123.72	118.28
1	A	258	LLP	C5-C6-N1	-4.28	116.86	123.83
1	A	258	LLP	OP4-C5'-C5	4.27	117.35	109.36
1	A	258	LLP	C6-N1-C2	4.19	126.80	119.20
1	A	258	LLP	C5'-C5-C6	-3.97	112.89	119.36
1	A	258	LLP	C2'-C2-C3	2.97	124.28	120.80
1	A	258	LLP	OP2-P-OP4	-2.95	98.99	106.67
1	A	258	LLP	O3-C3-C4	2.85	127.13	119.44
1	A	258	LLP	OP4-P-OP1	2.24	112.49	106.44
1	A	258	LLP	C3-C2-N1	-2.20	118.19	120.96

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	258	LLP	C4-C4'-NZ-CE
1	A	258	LLP	C4-C5-C5'-OP4
1	A	258	LLP	C6-C5-C5'-OP4
1	A	258	LLP	C5'-OP4-P-OP1
1	A	258	LLP	C5'-OP4-P-OP2
1	A	258	LLP	C5'-OP4-P-OP3
1	A	258	LLP	N-CA-CB-CG
1	A	258	LLP	C-CA-CB-CG
1	A	258	LLP	C3-C4-C4'-NZ
1	A	258	LLP	CA-CB-CG-CD
1	A	258	LLP	CE-CD-CG-CB
1	A	258	LLP	CG-CD-CE-NZ
1	A	258	LLP	C5-C4-C4'-NZ

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	258	LLP	7	0

5.5 Carbohydrates ⓘ

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	SO4	A	410	-	4,4,4	0.74	0	6,6,6	0.34	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.