



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:39 AM UTC

PDB ID : 3D1V / pdb_00003d1v
Title : Crystal structure of human PNP complexed with 2-mercapto(3H) quinazolinone
Authors : De Azevedo Jr., W.F.; Basso, L.A.; Santos, D.S.
Deposited on : 2008-05-06
Resolution : 2.70 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

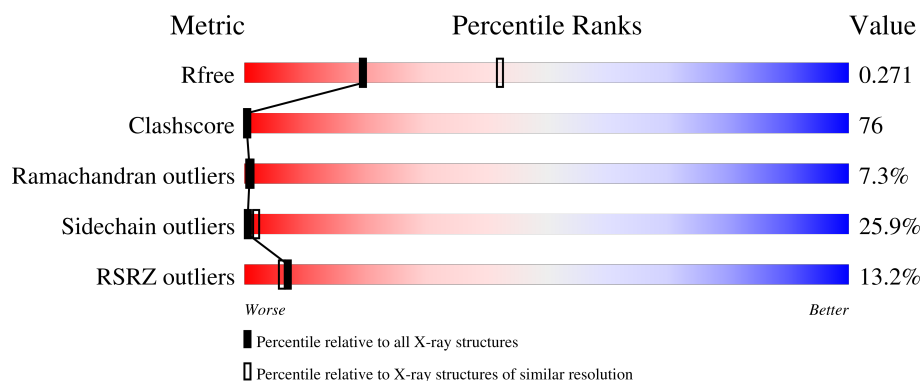
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	289	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	290	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	292	-	-	X	-
3	D1V	A	293	-	X	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2347 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.

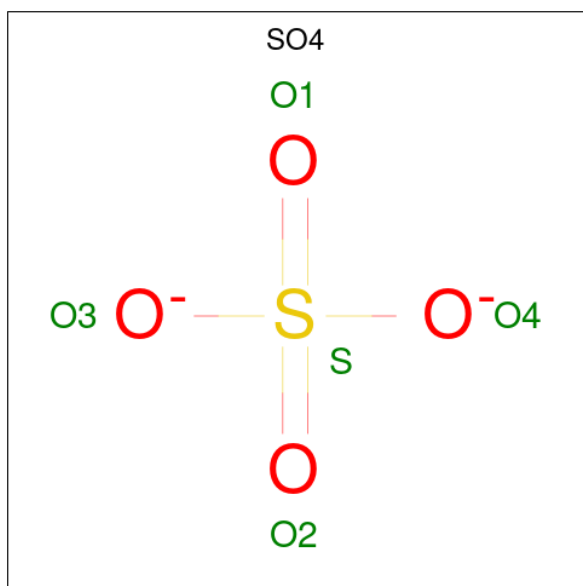
- Molecule 1 is a protein called Purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2251	1429	394	413	15	0	0	0

There is a discrepancy between the modelled and reference sequences:

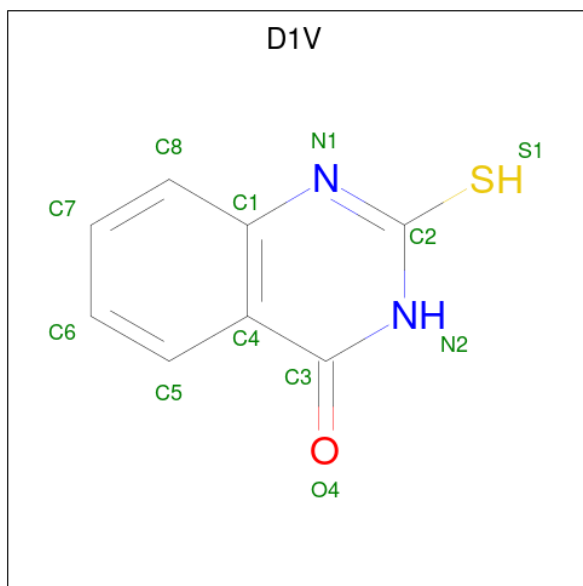
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	SER	GLY	conflict	UNP P00491

- 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
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

- Molecule 3 is 2-mercapto(3H)quinazolinone (CCD ID: D1V) (formula: C₈H₆N₂OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	12	8	2	1	1	0	0

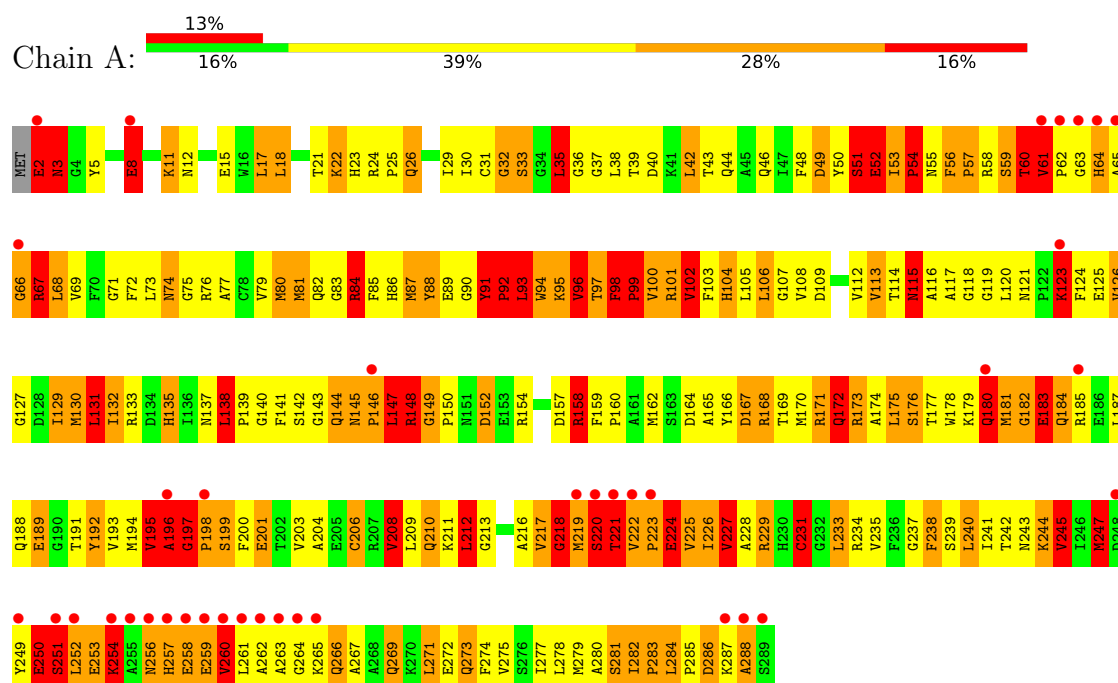
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	69	69	69	0	0

3 Residue-property plots [i](#)

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

• Molecule 1: Purine nucleoside phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	138.67Å 138.67Å 159.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.18 – 2.70 42.18 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (42.18-2.70) 98.7 (42.18-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.20 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.277 0.213 , 0.271	Depositor DCC
R_{free} test set	816 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 67.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2347	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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: SO4, D1V

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	3.95	178/2303 (7.7%)	2.94	215/3115 (6.9%)

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	20

All (178) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	PRO	N-CA	54.72	2.17	1.47
1	A	221	THR	C-O	53.81	1.91	1.24
1	A	146	PRO	C-N	43.39	1.92	1.33
1	A	197	GLY	N-CA	36.41	1.94	1.44
1	A	223	PRO	N-CD	33.79	1.95	1.47
1	A	220	SER	C-O	28.76	1.60	1.24
1	A	223	PRO	CA-CB	-27.53	1.14	1.53
1	A	196	ALA	N-CA	27.16	1.81	1.45
1	A	221	THR	CB-OG1	26.36	1.85	1.43
1	A	198	PRO	C-N	24.51	1.68	1.33
1	A	2	GLU	CD-OE1	23.66	1.70	1.25
1	A	221	THR	CB-CG2	22.69	2.27	1.52
1	A	146	PRO	C-O	21.19	1.52	1.24
1	A	220	SER	CA-C	19.84	1.79	1.52
1	A	196	ALA	C-N	19.82	1.63	1.33
1	A	94	TRP	N-CA	18.89	1.68	1.46
1	A	199	SER	CB-OG	17.65	1.77	1.42
1	A	147	LEU	C-O	17.15	1.48	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	VAL	N-CA	16.91	1.66	1.46
1	A	223	PRO	CA-C	16.76	1.76	1.52
1	A	224	GLU	N-CA	16.05	1.65	1.46
1	A	222	VAL	CA-CB	-15.97	1.33	1.54
1	A	219	MET	C-O	-15.82	1.12	1.23
1	A	225	VAL	C-O	15.73	1.41	1.24
1	A	198	PRO	CA-C	15.65	1.74	1.52
1	A	195	VAL	C-N	15.24	1.54	1.33
1	A	147	LEU	N-CA	-14.32	1.28	1.46
1	A	91	TYR	CA-CB	13.40	1.73	1.53
1	A	219	MET	CA-C	13.29	1.64	1.52
1	A	149	GLY	N-CA	13.08	1.62	1.44
1	A	195	VAL	C-O	12.98	1.39	1.24
1	A	97	THR	C-N	12.93	1.60	1.33
1	A	223	PRO	C-N	-12.07	1.18	1.33
1	A	97	THR	C-O	11.79	1.39	1.24
1	A	55	ASN	N-CA	11.72	1.60	1.46
1	A	219	MET	N-CA	11.68	1.57	1.47
1	A	222	VAL	CB-CG2	-11.40	1.15	1.52
1	A	148	ARG	CG-CD	11.22	1.86	1.52
1	A	196	ALA	CA-CB	11.14	1.71	1.53
1	A	94	TRP	CD2-CE3	11.14	1.58	1.40
1	A	61	VAL	N-CA	11.03	1.60	1.46
1	A	93	LEU	C-O	10.94	1.38	1.24
1	A	219	MET	CA-CB	10.83	1.75	1.53
1	A	92	PRO	N-CD	10.58	1.62	1.47
1	A	97	THR	CB-OG1	10.14	1.59	1.43
1	A	149	GLY	C-O	9.88	1.37	1.24
1	A	146	PRO	N-CA	9.87	1.59	1.47
1	A	61	VAL	CA-C	9.76	1.63	1.52
1	A	224	GLU	CA-C	-9.68	1.40	1.52
1	A	93	LEU	CB-CG	9.67	1.72	1.53
1	A	226	ILE	N-CA	9.56	1.57	1.46
1	A	220	SER	C-N	-9.56	1.20	1.33
1	A	222	VAL	C-O	9.55	1.36	1.24
1	A	218	GLY	C-N	9.40	1.51	1.34
1	A	219	MET	C-N	-9.38	1.20	1.33
1	A	198	PRO	N-CD	9.12	1.60	1.47
1	A	192	TYR	CA-CB	-9.09	1.41	1.53
1	A	92	PRO	C-O	9.05	1.35	1.23
1	A	141	PHE	C-O	8.99	1.35	1.24
1	A	129	ILE	CA-CB	-8.95	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	ILE	CB-CG1	8.94	1.71	1.53
1	A	147	LEU	CG-CD2	8.88	1.81	1.52
1	A	93	LEU	CA-C	-8.86	1.39	1.52
1	A	92	PRO	N-CA	-8.85	1.37	1.47
1	A	91	TYR	C-O	8.80	1.34	1.23
1	A	223	PRO	C-O	8.74	1.35	1.24
1	A	221	THR	CA-CB	-8.72	1.38	1.53
1	A	225	VAL	CA-CB	-8.65	1.44	1.54
1	A	98	PHE	CA-CB	8.53	1.67	1.53
1	A	57	PRO	C-O	-8.51	1.13	1.23
1	A	197	GLY	CA-C	-8.43	1.39	1.51
1	A	224	GLU	C-O	8.43	1.33	1.24
1	A	48	PHE	CA-C	-8.35	1.42	1.52
1	A	117	ALA	CA-CB	-8.21	1.39	1.53
1	A	148	ARG	CZ-NH2	8.09	1.44	1.33
1	A	227	VAL	CA-C	-8.09	1.42	1.53
1	A	92	PRO	CA-C	-8.06	1.43	1.52
1	A	195	VAL	CA-CB	-7.95	1.43	1.54
1	A	225	VAL	C-N	7.88	1.43	1.34
1	A	98	PHE	N-CA	-7.74	1.35	1.46
1	A	96	VAL	C-O	-7.73	1.14	1.24
1	A	94	TRP	C-O	7.68	1.34	1.24
1	A	91	TYR	CA-C	7.67	1.63	1.53
1	A	97	THR	CB-CG2	7.59	1.77	1.52
1	A	88	TYR	N-CA	7.53	1.56	1.46
1	A	97	THR	CA-CB	-7.53	1.42	1.53
1	A	61	VAL	CA-CB	7.41	1.63	1.54
1	A	54	PRO	C-O	7.38	1.33	1.24
1	A	238	PHE	CA-C	-7.38	1.43	1.52
1	A	219	MET	CG-SD	-7.36	1.62	1.80
1	A	195	VAL	N-CA	-7.32	1.37	1.46
1	A	53	ILE	N-CA	-7.31	1.41	1.46
1	A	113	VAL	C-O	-7.25	1.16	1.24
1	A	69	VAL	CA-CB	-7.18	1.45	1.54
1	A	146	PRO	CA-C	7.06	1.63	1.52
1	A	233	LEU	C-O	-6.96	1.15	1.23
1	A	81	MET	CA-C	-6.90	1.44	1.52
1	A	98	PHE	CG-CD1	-6.88	1.24	1.38
1	A	2	GLU	CB-CG	6.88	1.73	1.52
1	A	72	PHE	CA-C	-6.80	1.44	1.52
1	A	222	VAL	CA-C	6.78	1.60	1.52
1	A	198	PRO	N-CA	-6.77	1.38	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	PHE	CD2-CE2	6.66	1.58	1.38
1	A	31	CYS	C-O	-6.64	1.15	1.23
1	A	147	LEU	CA-CB	-6.63	1.43	1.53
1	A	2	GLU	N-CA	6.59	1.58	1.46
1	A	65	ALA	CA-C	6.57	1.64	1.52
1	A	59	SER	N-CA	6.52	1.53	1.46
1	A	152	ASP	CA-C	-6.47	1.44	1.52
1	A	66	GLY	N-CA	6.46	1.54	1.45
1	A	68	LEU	N-CA	-6.46	1.38	1.46
1	A	46	GLN	CA-C	6.46	1.60	1.52
1	A	98	PHE	CB-CG	-6.44	1.35	1.50
1	A	138	LEU	C-O	-6.44	1.18	1.24
1	A	2	GLU	CA-C	6.44	1.66	1.52
1	A	260	VAL	CA-CB	6.43	1.63	1.54
1	A	2	GLU	CD-OE2	6.43	1.37	1.25
1	A	53	ILE	CA-CB	-6.42	1.47	1.53
1	A	222	VAL	N-CA	6.42	1.54	1.46
1	A	114	THR	C-O	-6.40	1.15	1.23
1	A	95	LYS	CA-C	-6.36	1.44	1.52
1	A	220	SER	CB-OG	6.34	1.54	1.42
1	A	226	ILE	CA-CB	-6.32	1.46	1.54
1	A	64	HIS	CA-C	6.27	1.61	1.52
1	A	116	ALA	CA-C	-6.27	1.45	1.52
1	A	91	TYR	C-N	-6.23	1.25	1.33
1	A	3	ASN	N-CA	6.23	1.54	1.46
1	A	221	THR	C-N	-6.22	1.26	1.33
1	A	54	PRO	N-CA	-6.21	1.39	1.47
1	A	88	TYR	CA-C	6.17	1.61	1.52
1	A	102	VAL	CA-CB	6.16	1.61	1.54
1	A	201	GLU	CA-C	-6.14	1.44	1.53
1	A	33	SER	CA-C	-6.11	1.44	1.52
1	A	239	SER	N-CA	-6.09	1.38	1.46
1	A	94	TRP	CZ3-CH2	6.08	1.55	1.40
1	A	223	PRO	CB-CG	6.08	1.80	1.49
1	A	282	ILE	CA-CB	6.08	1.62	1.54
1	A	74	ASN	CA-C	-6.02	1.45	1.53
1	A	144	GLN	CB-CG	-6.02	1.34	1.52
1	A	206	CYS	C-O	5.99	1.30	1.24
1	A	254	LYS	N-CA	5.97	1.55	1.47
1	A	87	MET	C-O	-5.96	1.16	1.24
1	A	221	THR	CA-C	5.79	1.60	1.52
1	A	98	PHE	CG-CD2	-5.76	1.26	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	LEU	N-CA	5.74	1.53	1.46
1	A	219	MET	SD-CE	-5.68	1.65	1.79
1	A	254	LYS	CA-C	5.68	1.59	1.53
1	A	145	ASN	C-O	-5.65	1.16	1.24
1	A	65	ALA	C-N	5.63	1.41	1.33
1	A	91	TYR	N-CA	5.62	1.54	1.45
1	A	92	PRO	CG-CD	5.58	1.69	1.50
1	A	55	ASN	CA-C	-5.53	1.45	1.52
1	A	231	CYS	CB-SG	-5.52	1.63	1.81
1	A	35	LEU	CA-C	-5.51	1.45	1.52
1	A	198	PRO	C-O	5.49	1.31	1.24
1	A	99	PRO	CB-CG	5.46	1.76	1.49
1	A	115	ASN	CG-OD1	5.46	1.33	1.23
1	A	81	MET	N-CA	-5.45	1.39	1.46
1	A	67	ARG	N-CA	5.44	1.52	1.45
1	A	86	HIS	N-CA	-5.43	1.39	1.45
1	A	132	ILE	CA-CB	5.42	1.60	1.54
1	A	123	LYS	CG-CD	5.39	1.68	1.52
1	A	11	LYS	CG-CD	5.32	1.68	1.52
1	A	94	TRP	CG-CD2	5.31	1.53	1.43
1	A	220	SER	N-CA	-5.31	1.39	1.46
1	A	159	PHE	CD1-CE1	5.30	1.54	1.38
1	A	64	HIS	C-O	5.30	1.31	1.24
1	A	99	PRO	N-CA	-5.24	1.40	1.47
1	A	123	LYS	CD-CE	5.21	1.68	1.52
1	A	210	GLN	C-O	-5.21	1.18	1.24
1	A	60	THR	C-N	5.19	1.39	1.33
1	A	98	PHE	CD1-CE1	5.19	1.54	1.38
1	A	240	LEU	N-CA	-5.12	1.39	1.46
1	A	280	ALA	CA-CB	-5.08	1.45	1.53
1	A	53	ILE	CA-C	-5.06	1.49	1.53
1	A	148	ARG	CZ-NH1	-5.05	1.25	1.32
1	A	145	ASN	N-CA	5.04	1.54	1.45
1	A	8	GLU	CA-C	-5.01	1.46	1.52

All (215) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	THR	CA-CB-OG1	-26.28	70.19	109.60
1	A	196	ALA	CA-C-N	-23.34	85.22	121.87
1	A	196	ALA	C-N-CA	-23.34	85.22	121.87
1	A	91	TYR	CA-C-N	-22.39	98.36	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	TYR	C-N-CA	-22.39	98.36	120.52
1	A	223	PRO	N-CD-CG	-19.81	73.48	103.20
1	A	219	MET	O-C-N	-19.16	104.03	121.85
1	A	221	THR	N-CA-C	18.96	151.19	110.80
1	A	54	PRO	CA-C-N	-18.21	94.33	122.37
1	A	54	PRO	C-N-CA	-18.21	94.33	122.37
1	A	97	THR	N-CA-C	-18.19	92.56	112.93
1	A	97	THR	CA-CB-OG1	-16.07	85.49	109.60
1	A	146	PRO	CA-C-O	15.79	139.84	118.99
1	A	223	PRO	CA-N-CD	-15.18	90.74	112.00
1	A	93	LEU	CA-C-N	-14.83	99.10	122.67
1	A	93	LEU	C-N-CA	-14.83	99.10	122.67
1	A	148	ARG	CA-C-O	-14.58	105.55	122.03
1	A	92	PRO	N-CA-C	14.55	132.81	111.13
1	A	195	VAL	CA-C-O	13.85	138.99	121.40
1	A	148	ARG	NE-CZ-NH2	13.55	131.40	119.20
1	A	91	TYR	CA-C-O	-12.82	106.77	120.87
1	A	219	MET	CA-C-N	12.58	145.57	121.54
1	A	219	MET	C-N-CA	12.58	145.57	121.54
1	A	118	GLY	N-CA-C	-12.30	88.81	110.71
1	A	198	PRO	O-C-N	-12.23	106.13	122.64
1	A	92	PRO	CA-C-O	-11.71	106.69	122.15
1	A	196	ALA	CA-C-O	11.19	134.81	121.94
1	A	94	TRP	N-CA-C	-11.08	99.07	112.59
1	A	98	PHE	CA-C-O	-10.90	105.22	120.16
1	A	227	VAL	CB-CA-C	10.89	127.00	111.65
1	A	222	VAL	O-C-N	-10.66	108.94	121.10
1	A	97	THR	CB-CA-C	10.61	129.17	110.81
1	A	199	SER	CA-CB-OG	-10.43	90.24	111.10
1	A	222	VAL	CB-CA-C	-10.40	92.43	111.36
1	A	88	TYR	N-CA-C	-10.27	100.01	112.54
1	A	61	VAL	N-CA-C	10.26	131.03	108.88
1	A	98	PHE	CA-CB-CG	-10.24	103.56	113.80
1	A	197	GLY	CA-C-N	-10.21	107.08	119.84
1	A	197	GLY	C-N-CA	-10.21	107.08	119.84
1	A	225	VAL	CA-C-O	-10.10	109.47	121.18
1	A	89	GLU	CA-C-N	-10.08	111.45	123.44
1	A	89	GLU	C-N-CA	-10.08	111.45	123.44
1	A	222	VAL	CA-CB-CG2	-9.98	93.44	110.40
1	A	89	GLU	N-CA-C	-9.84	101.28	113.28
1	A	147	LEU	N-CA-C	-9.55	99.48	112.94
1	A	223	PRO	N-CA-CB	-9.45	93.33	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ALA	N-CA-C	-9.43	98.36	110.53
1	A	2	GLU	CG-CD-OE1	-9.36	96.88	118.40
1	A	142	SER	N-CA-C	9.36	124.77	113.16
1	A	54	PRO	O-C-N	-9.13	110.32	122.64
1	A	288	ALA	N-CA-C	8.96	123.81	111.17
1	A	99	PRO	N-CA-C	-8.96	100.82	113.81
1	A	199	SER	CB-CA-C	8.93	128.19	110.42
1	A	224	GLU	CB-CA-C	8.88	125.01	110.81
1	A	196	ALA	O-C-N	-8.87	111.75	122.65
1	A	195	VAL	O-C-N	-8.85	113.78	122.98
1	A	90	GLY	CA-C-N	-8.83	106.90	121.03
1	A	90	GLY	C-N-CA	-8.83	106.90	121.03
1	A	80	MET	CG-SD-CE	-8.76	81.63	100.90
1	A	96	VAL	CA-C-O	-8.67	109.94	120.78
1	A	200	PHE	N-CA-CB	-8.66	97.26	110.42
1	A	219	MET	CG-SD-CE	8.65	119.94	100.90
1	A	98	PHE	CB-CA-C	8.64	127.20	110.17
1	A	229	ARG	N-CA-C	-8.61	101.83	111.82
1	A	2	GLU	CG-CD-OE2	8.59	138.17	118.40
1	A	183	GLU	N-CA-C	8.45	122.85	109.50
1	A	52	GLU	CA-C-N	-8.40	116.54	122.59
1	A	52	GLU	C-N-CA	-8.40	116.54	122.59
1	A	217	VAL	CA-C-N	-8.31	113.03	122.42
1	A	217	VAL	C-N-CA	-8.31	113.03	122.42
1	A	93	LEU	N-CA-C	-8.25	101.62	112.34
1	A	219	MET	N-CA-CB	8.22	124.72	110.65
1	A	168	ARG	N-CA-C	-8.14	102.36	111.07
1	A	220	SER	CA-C-N	-8.12	106.03	121.54
1	A	220	SER	C-N-CA	-8.12	106.03	121.54
1	A	226	ILE	CA-C-O	-8.10	112.63	121.05
1	A	217	VAL	CA-C-O	8.08	129.05	120.48
1	A	149	GLY	CA-C-N	8.00	127.95	120.03
1	A	149	GLY	C-N-CA	8.00	127.95	120.03
1	A	147	LEU	CA-C-N	-7.94	106.82	120.95
1	A	147	LEU	C-N-CA	-7.94	106.82	120.95
1	A	225	VAL	O-C-N	7.91	130.41	121.94
1	A	120	LEU	N-CA-C	-7.84	103.56	113.43
1	A	257	HIS	N-CA-C	7.81	119.58	111.14
1	A	148	ARG	CA-C-N	7.66	133.89	121.87
1	A	148	ARG	C-N-CA	7.66	133.89	121.87
1	A	223	PRO	CA-C-O	-7.64	106.70	120.60
1	A	75	GLY	N-CA-C	-7.57	95.25	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	GLY	CA-C-N	-7.56	106.65	119.35
1	A	218	GLY	C-N-CA	-7.56	106.65	119.35
1	A	195	VAL	CA-C-N	-7.54	105.31	121.45
1	A	195	VAL	C-N-CA	-7.54	105.31	121.45
1	A	92	PRO	N-CD-CG	-7.52	91.92	103.20
1	A	56	PHE	CA-C-N	-7.45	112.30	119.90
1	A	56	PHE	C-N-CA	-7.45	112.30	119.90
1	A	90	GLY	O-C-N	-7.45	115.77	122.77
1	A	149	GLY	O-C-N	-7.41	114.36	121.77
1	A	32	GLY	N-CA-C	-7.25	102.80	112.81
1	A	93	LEU	CB-CA-C	7.21	126.33	110.18
1	A	92	PRO	CA-CB-CG	-7.16	90.90	104.50
1	A	226	ILE	CB-CA-C	7.16	121.41	112.04
1	A	223	PRO	CA-C-N	7.14	130.19	120.54
1	A	223	PRO	C-N-CA	7.14	130.19	120.54
1	A	221	THR	N-CA-CB	-7.14	98.43	110.49
1	A	148	ARG	CB-CG-CD	7.09	127.61	111.30
1	A	254	LYS	N-CA-C	7.08	122.02	107.37
1	A	192	TYR	N-CA-CB	-7.05	98.92	110.42
1	A	102	VAL	N-CA-CB	7.03	119.57	110.57
1	A	94	TRP	O-C-N	6.99	130.86	122.26
1	A	199	SER	CA-C-O	-6.97	110.54	120.51
1	A	93	LEU	CD1-CG-CD2	6.95	126.09	110.80
1	A	226	ILE	CA-CB-CG1	-6.95	98.59	110.40
1	A	60	THR	N-CA-C	6.94	121.92	113.17
1	A	208	VAL	N-CA-C	6.91	118.49	110.62
1	A	145	ASN	CA-C-N	6.89	127.77	120.12
1	A	145	ASN	C-N-CA	6.89	127.77	120.12
1	A	99	PRO	CB-CG-CD	-6.88	84.08	106.10
1	A	208	VAL	N-CA-CB	6.85	119.03	110.47
1	A	158	ARG	CA-C-N	-6.84	114.87	123.15
1	A	158	ARG	C-N-CA	-6.84	114.87	123.15
1	A	144	GLN	CA-C-O	-6.80	114.14	122.64
1	A	199	SER	N-CA-C	-6.80	96.32	110.80
1	A	127	GLY	N-CA-C	-6.78	105.86	113.79
1	A	91	TYR	N-CA-CB	-6.73	100.36	110.05
1	A	148	ARG	CD-NE-CZ	-6.71	115.00	124.40
1	A	131	LEU	CA-C-N	-6.71	112.41	121.80
1	A	131	LEU	C-N-CA	-6.71	112.41	121.80
1	A	218	GLY	CA-C-O	6.71	129.64	120.92
1	A	147	LEU	CB-CG-CD2	6.63	130.60	110.70
1	A	146	PRO	O-C-N	-6.59	111.16	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	SER	CB-CA-C	-6.58	98.45	113.33
1	A	150	PRO	CB-CA-C	-6.39	102.58	110.95
1	A	90	GLY	N-CA-C	6.35	121.22	113.79
1	A	37	GLY	N-CA-C	-6.33	104.94	113.24
1	A	206	CYS	CA-CB-SG	-6.25	100.01	114.40
1	A	218	GLY	O-C-N	-6.22	115.01	123.16
1	A	18	LEU	N-CA-C	-6.21	104.20	110.97
1	A	224	GLU	N-CA-CB	-6.14	100.79	109.94
1	A	220	SER	CA-C-O	-6.12	111.76	120.51
1	A	219	MET	CB-CA-C	-6.10	96.97	110.99
1	A	147	LEU	CB-CA-C	-6.07	100.19	110.64
1	A	191	THR	CA-C-O	6.07	127.61	120.69
1	A	148	ARG	NH1-CZ-NH2	-6.06	111.42	119.30
1	A	204	ALA	N-CA-C	-6.06	104.79	111.82
1	A	98	PHE	N-CA-C	-6.05	96.43	109.81
1	A	69	VAL	CB-CA-C	-6.02	102.17	110.96
1	A	245	VAL	N-CA-C	-6.01	99.74	108.87
1	A	100	VAL	CA-C-O	6.00	126.95	120.47
1	A	97	THR	CA-C-O	-5.95	112.27	119.59
1	A	198	PRO	CA-C-O	-5.94	109.79	120.60
1	A	8	GLU	N-CA-CB	5.89	118.78	110.12
1	A	221	THR	OG1-CB-CG2	-5.89	97.53	109.30
1	A	221	THR	CB-CA-C	-5.88	98.72	110.42
1	A	279	MET	CA-C-N	5.87	128.63	120.29
1	A	279	MET	C-N-CA	5.87	128.63	120.29
1	A	51	SER	N-CA-CB	-5.85	100.60	110.49
1	A	281	SER	CA-C-N	-5.81	111.38	122.13
1	A	281	SER	C-N-CA	-5.81	111.38	122.13
1	A	91	TYR	O-C-N	5.77	127.72	121.60
1	A	96	VAL	N-CA-CB	-5.77	101.72	111.23
1	A	220	SER	O-C-N	5.73	130.21	122.59
1	A	200	PHE	N-CA-C	-5.70	102.32	110.59
1	A	143	GLY	CA-C-O	5.70	130.48	120.57
1	A	91	TYR	C-N-CD	5.68	148.29	125.00
1	A	195	VAL	N-CA-C	-5.68	100.26	108.89
1	A	2	GLU	N-CA-C	5.66	126.84	111.00
1	A	130	MET	CA-C-N	-5.66	114.92	122.72
1	A	130	MET	C-N-CA	-5.66	114.92	122.72
1	A	203	VAL	N-CA-C	-5.64	105.02	110.72
1	A	146	PRO	CA-C-N	-5.62	113.72	122.37
1	A	146	PRO	C-N-CA	-5.62	113.72	122.37
1	A	212	LEU	N-CA-C	-5.61	105.70	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	SER	N-CA-C	5.58	122.68	110.80
1	A	171	ARG	N-CA-C	-5.57	105.29	111.36
1	A	192	TYR	CA-C-N	-5.57	115.41	122.37
1	A	192	TYR	C-N-CA	-5.57	115.41	122.37
1	A	234	ARG	CA-C-N	-5.56	115.39	123.06
1	A	234	ARG	C-N-CA	-5.56	115.39	123.06
1	A	231	CYS	N-CA-CB	-5.55	101.78	110.44
1	A	135	HIS	CA-C-N	-5.53	115.90	123.14
1	A	135	HIS	C-N-CA	-5.53	115.90	123.14
1	A	197	GLY	CA-C-O	-5.51	113.64	121.52
1	A	237	GLY	N-CA-C	5.50	118.56	110.80
1	A	224	GLU	CA-C-O	-5.49	115.02	120.90
1	A	80	MET	N-CA-C	5.48	118.67	109.95
1	A	91	TYR	CB-CA-C	-5.47	99.40	109.51
1	A	224	GLU	O-C-N	5.45	127.76	122.09
1	A	97	THR	CA-C-N	-5.44	108.53	121.80
1	A	97	THR	C-N-CA	-5.44	108.53	121.80
1	A	222	VAL	N-CA-C	-5.37	97.28	108.88
1	A	219	MET	CB-CG-SD	5.35	128.75	112.70
1	A	84	ARG	CA-C-N	5.30	129.00	121.42
1	A	84	ARG	C-N-CA	5.30	129.00	121.42
1	A	217	VAL	CB-CA-C	-5.30	102.93	110.83
1	A	30	ILE	N-CA-C	-5.27	99.97	107.77
1	A	225	VAL	CG1-CB-CG2	-5.26	99.22	110.80
1	A	67	ARG	N-CA-C	5.25	117.17	109.24
1	A	244	LYS	N-CA-C	-5.25	100.17	108.73
1	A	216	ALA	N-CA-C	-5.24	100.86	109.40
1	A	101	ARG	N-CA-C	-5.23	106.41	112.89
1	A	17	LEU	N-CA-C	-5.22	106.06	112.90
1	A	74	ASN	CB-CA-C	-5.22	104.86	111.86
1	A	83	GLY	N-CA-C	-5.21	100.83	113.18
1	A	98	PHE	CE1-CZ-CE2	-5.20	110.65	120.00
1	A	197	GLY	N-CA-C	-5.17	101.80	112.34
1	A	42	LEU	CA-C-N	-5.16	114.38	122.73
1	A	42	LEU	C-N-CA	-5.16	114.38	122.73
1	A	251	SER	N-CA-C	5.14	121.75	110.80
1	A	3	ASN	N-CA-C	5.11	121.68	110.80
1	A	123	LYS	CA-CB-CG	5.07	124.25	114.10
1	A	114	THR	CA-C-O	-5.04	115.73	121.68
1	A	99	PRO	CA-CB-CG	-5.03	94.94	104.50
1	A	142	SER	CA-C-O	-5.01	113.22	119.28
1	A	36	GLY	N-CA-C	-5.00	108.45	114.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	VAL	CB-CA-C	-5.00	104.16	112.26

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	LEU	Mainchain
1	A	183	GLU	Peptide
1	A	189	GLU	Peptide
1	A	196	ALA	Peptide
1	A	197	GLY	Peptide,Mainchain
1	A	218	GLY	Mainchain
1	A	220	SER	Mainchain
1	A	221	THR	Mainchain
1	A	224	GLU	Mainchain
1	A	247	MET	Peptide
1	A	286	ASP	Peptide
1	A	50	TYR	Peptide
1	A	60	THR	Peptide
1	A	61	VAL	Peptide
1	A	64	HIS	Peptide
1	A	73	LEU	Peptide
1	A	91	TYR	Mainchain
1	A	96	VAL	Peptide
1	A	98	PHE	Mainchain

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	2251	0	2220	342	0
2	A	15	0	0	5	0
3	A	12	0	6	5	0
4	A	69	0	0	7	0
All	All	2347	0	2226	342	0

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 76.

All (342) 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:198:PRO:C	1:A:198:PRO:CA	1.74	1.58
1:A:147:LEU:CD2	1:A:147:LEU:CG	1.81	1.57
1:A:223:PRO:CG	1:A:223:PRO:CB	1.80	1.57
1:A:223:PRO:C	1:A:223:PRO:CA	1.76	1.56
1:A:97:THR:CG2	1:A:97:THR:CB	1.77	1.56
1:A:220:SER:C	1:A:220:SER:CA	1.79	1.55
1:A:148:ARG:CG	1:A:148:ARG:CD	1.86	1.54
1:A:219:MET:CB	1:A:219:MET:CA	1.74	1.54
1:A:99:PRO:CG	1:A:99:PRO:CB	1.77	1.53
1:A:94:TRP:N	1:A:94:TRP:CA	1.68	1.50
1:A:198:PRO:C	1:A:199:SER:N	1.68	1.50
1:A:196:ALA:N	1:A:196:ALA:CA	1.81	1.42
1:A:2:GLU:OE1	1:A:2:GLU:CD	1.70	1.32
1:A:199:SER:OG	1:A:199:SER:CB	1.77	1.32
1:A:197:GLY:CA	1:A:197:GLY:N	1.94	1.30
1:A:223:PRO:N	1:A:223:PRO:CD	1.95	1.28
1:A:22:LYS:CE	1:A:22:LYS:HA	1.61	1.28
1:A:146:PRO:C	1:A:147:LEU:N	1.91	1.28
1:A:148:ARG:NH1	2:A:292:SO4:O1	1.79	1.16
1:A:221:THR:O	1:A:221:THR:C	1.91	1.13
1:A:146:PRO:HG3	1:A:223:PRO:HA	1.19	1.13
1:A:221:THR:CB	1:A:221:THR:CG2	2.27	1.11
1:A:243:ASN:ND2	1:A:256:ASN:HA	1.65	1.10
1:A:243:ASN:HD21	1:A:256:ASN:HA	0.98	1.10
1:A:42:LEU:HD22	1:A:71:GLY:HA3	1.14	1.10
1:A:22:LYS:HA	1:A:22:LYS:HE3	1.15	1.08
1:A:223:PRO:CG	1:A:223:PRO:N	2.16	1.08
1:A:223:PRO:CA	1:A:223:PRO:N	2.17	1.07
1:A:249:TYR:O	1:A:250:GLU:HG3	1.58	1.03
1:A:93:LEU:C	1:A:94:TRP:CA	2.31	1.02
1:A:147:LEU:HD22	1:A:226:ILE:HG22	1.49	0.95
1:A:247:MET:HE3	1:A:247:MET:HA	1.48	0.94
1:A:223:PRO:CB	1:A:223:PRO:C	2.41	0.94
1:A:22:LYS:CE	1:A:22:LYS:CA	2.47	0.92
1:A:196:ALA:C	1:A:197:GLY:CA	2.43	0.91
1:A:22:LYS:HE3	1:A:22:LYS:CA	2.00	0.91
1:A:201:GLU:CD	3:A:293:D1V:S1	2.55	0.90
1:A:223:PRO:CG	1:A:223:PRO:CA	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ASN:HD21	1:A:256:ASN:CA	1.84	0.89
1:A:223:PRO:CB	1:A:223:PRO:CD	2.50	0.89
1:A:22:LYS:HA	1:A:22:LYS:HE2	1.51	0.89
1:A:201:GLU:OE1	3:A:293:D1V:S1	2.30	0.89
1:A:223:PRO:O	1:A:227:VAL:HG13	1.72	0.89
1:A:284:LEU:HD23	1:A:288:ALA:O	1.73	0.89
1:A:167:ASP:O	1:A:171:ARG:HD3	1.73	0.88
1:A:201:GLU:CD	3:A:293:D1V:HS1	1.80	0.88
1:A:97:THR:HG21	1:A:146:PRO:HB3	1.54	0.87
1:A:49:ASP:OD1	1:A:51:SER:OG	1.92	0.86
1:A:42:LEU:HD22	1:A:71:GLY:CA	2.02	0.85
1:A:147:LEU:CD2	1:A:147:LEU:HG	2.04	0.83
1:A:196:ALA:O	1:A:197:GLY:O	1.96	0.82
1:A:219:MET:CB	1:A:219:MET:C	2.54	0.81
1:A:146:PRO:CG	1:A:223:PRO:HA	2.07	0.81
1:A:100:VAL:HG21	1:A:224:GLU:HA	1.61	0.81
1:A:88:TYR:HB2	1:A:198:PRO:HB3	1.61	0.81
1:A:264:GLY:CA	4:A:349:HOH:O	2.28	0.81
1:A:264:GLY:HA2	4:A:349:HOH:O	1.81	0.81
1:A:94:TRP:N	1:A:94:TRP:C	2.39	0.80
1:A:179:LYS:O	1:A:182:GLY:N	2.10	0.79
1:A:220:SER:C	1:A:220:SER:CB	2.55	0.78
1:A:97:THR:CG2	1:A:97:THR:CA	2.59	0.78
1:A:199:SER:OG	1:A:199:SER:CA	2.32	0.77
1:A:222:VAL:O	1:A:226:ILE:HG13	1.83	0.77
1:A:201:GLU:OE1	1:A:201:GLU:N	2.15	0.77
1:A:42:LEU:CD2	1:A:71:GLY:HA3	2.06	0.77
1:A:81:MET:CE	1:A:84:ARG:HA	2.14	0.77
1:A:49:ASP:HB3	1:A:51:SER:HB2	1.66	0.75
1:A:94:TRP:N	1:A:95:LYS:N	2.34	0.75
1:A:219:MET:CA	1:A:219:MET:CG	2.63	0.74
1:A:223:PRO:N	1:A:223:PRO:HG3	2.03	0.74
1:A:177:THR:HA	1:A:180:GLN:HG2	1.70	0.74
1:A:223:PRO:CB	1:A:223:PRO:N	2.51	0.73
1:A:79:VAL:O	1:A:79:VAL:HG13	1.88	0.73
1:A:148:ARG:NH1	2:A:292:SO4:S	2.60	0.72
1:A:38:LEU:HB2	1:A:272:GLU:HG2	1.72	0.72
1:A:60:THR:O	1:A:61:VAL:HB	1.90	0.71
1:A:146:PRO:HG2	1:A:226:ILE:HB	1.72	0.71
1:A:199:SER:N	1:A:199:SER:OG	2.22	0.71
1:A:157:ASP:O	1:A:160:PRO:HD3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:O	1:A:94:TRP:CA	2.39	0.71
1:A:198:PRO:C	1:A:198:PRO:CB	2.62	0.71
1:A:196:ALA:N	1:A:196:ALA:C	2.49	0.71
1:A:38:LEU:HD23	1:A:38:LEU:C	2.16	0.70
1:A:94:TRP:N	1:A:95:LYS:H	1.89	0.70
1:A:81:MET:HE2	1:A:84:ARG:HA	1.73	0.70
1:A:49:ASP:O	1:A:52:GLU:HG3	1.91	0.70
1:A:249:TYR:C	1:A:250:GLU:HG3	2.16	0.70
1:A:201:GLU:OE2	3:A:293:DIV:S1	2.50	0.70
1:A:63:GLY:O	1:A:66:GLY:HA3	1.91	0.69
1:A:147:LEU:N	1:A:147:LEU:HD13	2.07	0.69
1:A:93:LEU:O	1:A:94:TRP:HA	1.93	0.69
1:A:146:PRO:HB2	1:A:227:VAL:HG11	1.75	0.69
1:A:146:PRO:HB2	1:A:227:VAL:CG1	2.23	0.68
1:A:147:LEU:HD22	1:A:226:ILE:CG2	2.22	0.68
1:A:223:PRO:HD2	1:A:224:GLU:OE1	1.94	0.68
1:A:63:GLY:O	1:A:66:GLY:CA	2.41	0.68
1:A:38:LEU:HD23	1:A:38:LEU:O	1.94	0.67
1:A:195:VAL:C	1:A:196:ALA:CA	2.67	0.67
1:A:165:ALA:O	1:A:229:ARG:HD3	1.94	0.67
1:A:135:HIS:CE1	1:A:222:VAL:HG13	2.30	0.66
1:A:265:LYS:O	1:A:269:GLN:CG	2.44	0.66
1:A:38:LEU:CD2	1:A:80:MET:SD	2.84	0.65
1:A:129:ILE:HG22	1:A:130:MET:N	2.11	0.65
1:A:223:PRO:C	1:A:223:PRO:HB2	2.22	0.65
1:A:121:ASN:O	1:A:124:PHE:HB2	1.97	0.65
1:A:220:SER:CA	1:A:221:THR:N	2.51	0.65
1:A:104:HIS:O	1:A:107:GLY:N	2.29	0.65
1:A:133:ARG:CG	1:A:171:ARG:HH21	2.10	0.64
1:A:74:ASN:CG	1:A:74:ASN:O	2.37	0.64
1:A:113:VAL:HG21	1:A:221:THR:CG2	2.27	0.64
1:A:146:PRO:C	1:A:147:LEU:CA	2.70	0.64
1:A:109:ASP:HA	1:A:233:LEU:HD22	1.81	0.63
1:A:177:THR:HA	1:A:180:GLN:CG	2.28	0.63
1:A:29:ILE:HB	1:A:80:MET:HG2	1.79	0.63
1:A:252:LEU:H	1:A:252:LEU:HD12	1.62	0.63
1:A:252:LEU:H	1:A:252:LEU:CD1	2.11	0.63
1:A:92:PRO:C	1:A:94:TRP:N	2.51	0.63
1:A:210:GLN:NE2	1:A:247:MET:HE2	2.13	0.63
1:A:49:ASP:HB3	1:A:51:SER:CB	2.29	0.62
1:A:147:LEU:CD2	1:A:147:LEU:CD1	2.71	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:CD2	1:A:226:ILE:HG22	2.27	0.62
1:A:97:THR:HG22	1:A:223:PRO:HB2	1.81	0.62
1:A:240:LEU:HD11	1:A:267:ALA:HB1	1.81	0.62
1:A:97:THR:CG2	1:A:223:PRO:CB	2.77	0.62
1:A:131:LEU:HD11	1:A:171:ARG:HG2	1.83	0.61
1:A:271:LEU:HD22	1:A:275:VAL:HG23	1.83	0.61
1:A:2:GLU:OE1	1:A:2:GLU:CG	2.49	0.61
1:A:198:PRO:C	1:A:199:SER:O	2.44	0.61
1:A:76:ARG:NH2	1:A:282:ILE:O	2.32	0.61
1:A:210:GLN:HE21	1:A:247:MET:CE	2.13	0.61
1:A:210:GLN:NE2	1:A:247:MET:CE	2.64	0.60
1:A:97:THR:CG2	1:A:223:PRO:HB3	2.31	0.60
1:A:97:THR:HG21	1:A:146:PRO:CB	2.30	0.60
1:A:168:ARG:HG2	1:A:171:ARG:HH12	1.67	0.60
1:A:91:TYR:HB3	1:A:95:LYS:HB2	1.84	0.59
1:A:113:VAL:HG23	1:A:113:VAL:O	2.02	0.59
1:A:242:THR:HG21	1:A:257:HIS:ND1	2.18	0.59
1:A:167:ASP:HB3	1:A:170:MET:H	1.67	0.59
1:A:262:ALA:HB1	1:A:266:GLN:HB2	1.85	0.59
1:A:256:ASN:H	1:A:259:GLU:CD	2.11	0.58
1:A:265:LYS:O	1:A:269:GLN:HG3	2.02	0.58
1:A:92:PRO:C	1:A:94:TRP:H	2.11	0.58
1:A:84:ARG:NH1	2:A:290:SO4:O2	2.33	0.58
1:A:23:HIS:O	1:A:24:ARG:HD3	2.04	0.58
1:A:274:PHE:CZ	1:A:278:LEU:HD11	2.39	0.58
1:A:113:VAL:HG21	1:A:221:THR:HG23	1.85	0.58
1:A:178:TRP:CG	1:A:187:LEU:HB2	2.39	0.58
1:A:152:ASP:OD1	1:A:154:ARG:HB2	2.04	0.58
1:A:228:ALA:O	1:A:231:CYS:HB2	2.04	0.57
1:A:242:THR:OG1	1:A:257:HIS:HB2	2.05	0.57
1:A:174:ALA:HA	1:A:278:LEU:HD21	1.87	0.56
1:A:169:THR:O	1:A:172:GLN:HB3	2.05	0.56
1:A:38:LEU:HD22	1:A:80:MET:SD	2.46	0.56
1:A:129:ILE:CG2	1:A:130:MET:N	2.68	0.56
1:A:222:VAL:HG12	1:A:226:ILE:HD11	1.87	0.56
1:A:97:THR:CG2	1:A:146:PRO:HB3	2.30	0.56
1:A:187:LEU:CD1	1:A:274:PHE:HE2	2.19	0.56
1:A:187:LEU:CD1	1:A:274:PHE:CE2	2.89	0.56
1:A:131:LEU:HD23	1:A:238:PHE:CE1	2.41	0.55
1:A:11:LYS:HD2	1:A:15:GLU:OE1	2.05	0.55
1:A:67:ARG:NE	1:A:82:GLN:OE1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PHE:C	1:A:100:VAL:N	2.61	0.55
1:A:146:PRO:HG3	1:A:223:PRO:CA	2.13	0.55
1:A:220:SER:CB	1:A:221:THR:N	2.69	0.55
1:A:197:GLY:N	1:A:197:GLY:C	2.61	0.55
1:A:201:GLU:CD	1:A:201:GLU:N	2.64	0.55
1:A:84:ARG:NE	1:A:220:SER:HB2	2.22	0.55
1:A:149:GLY:O	1:A:158:ARG:NH2	2.31	0.55
1:A:177:THR:CA	1:A:180:GLN:HG2	2.36	0.55
1:A:91:TYR:HB3	1:A:95:LYS:CB	2.37	0.54
1:A:97:THR:HG21	1:A:223:PRO:HB3	1.88	0.54
1:A:56:PHE:O	1:A:57:PRO:C	2.47	0.54
1:A:79:VAL:O	1:A:79:VAL:CG1	2.55	0.54
1:A:99:PRO:O	1:A:100:VAL:C	2.49	0.54
1:A:32:GLY:H	1:A:35:LEU:HD12	1.72	0.54
1:A:144:GLN:OE1	1:A:144:GLN:HA	2.06	0.54
1:A:43:THR:O	1:A:44:GLN:HB2	2.07	0.54
1:A:63:GLY:O	1:A:66:GLY:N	2.40	0.54
1:A:96:VAL:C	1:A:98:PHE:N	2.64	0.54
1:A:57:PRO:HG3	1:A:95:LYS:HG2	1.90	0.53
1:A:2:GLU:OE1	1:A:147:LEU:O	2.26	0.53
1:A:3:ASN:C	1:A:5:TYR:H	2.16	0.53
1:A:63:GLY:C	1:A:66:GLY:H	2.16	0.53
1:A:223:PRO:CA	1:A:223:PRO:O	2.50	0.53
1:A:103:PHE:O	1:A:104:HIS:O	2.27	0.53
1:A:198:PRO:CA	1:A:198:PRO:O	2.51	0.53
1:A:247:MET:HE3	1:A:247:MET:CA	2.28	0.53
1:A:247:MET:HA	1:A:247:MET:CE	2.29	0.53
1:A:221:THR:O	1:A:222:VAL:C	2.52	0.53
1:A:252:LEU:HD12	1:A:252:LEU:N	2.23	0.52
1:A:97:THR:HG22	1:A:223:PRO:CB	2.37	0.52
1:A:265:LYS:O	1:A:269:GLN:HG2	2.09	0.52
1:A:262:ALA:O	1:A:266:GLN:HB2	2.09	0.52
1:A:103:PHE:O	1:A:104:HIS:C	2.53	0.52
1:A:222:VAL:O	1:A:222:VAL:HG12	2.08	0.52
1:A:133:ARG:HG3	1:A:171:ARG:HH21	1.74	0.52
1:A:225:VAL:HG13	1:A:235:VAL:HG11	1.92	0.51
1:A:139:PRO:HD3	1:A:194:MET:O	2.10	0.51
1:A:249:TYR:O	1:A:250:GLU:CG	2.46	0.51
1:A:22:LYS:CA	1:A:22:LYS:HE2	2.29	0.51
1:A:262:ALA:O	1:A:266:GLN:CB	2.59	0.51
1:A:162:MET:HE3	1:A:226:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLU:OE2	1:A:253:GLU:HG2	2.10	0.51
1:A:8:GLU:CD	1:A:8:GLU:H	2.19	0.51
1:A:11:LYS:O	1:A:12:ASN:C	2.52	0.51
1:A:58:ARG:HD2	4:A:346:HOH:O	2.10	0.50
1:A:119:GLY:O	1:A:245:VAL:HB	2.11	0.50
1:A:94:TRP:O	1:A:98:PHE:HB2	2.10	0.50
1:A:92:PRO:O	1:A:94:TRP:N	2.45	0.50
1:A:281:SER:O	1:A:283:PRO:CD	2.59	0.50
1:A:210:GLN:O	1:A:213:GLY:N	2.34	0.50
1:A:97:THR:CG2	1:A:97:THR:HB	2.20	0.50
1:A:146:PRO:C	1:A:147:LEU:HD13	2.37	0.50
1:A:113:VAL:CG2	1:A:221:THR:HG23	2.42	0.50
1:A:124:PHE:O	1:A:244:LYS:HE2	2.11	0.50
1:A:97:THR:HG21	1:A:223:PRO:CB	2.42	0.50
1:A:220:SER:O	1:A:222:VAL:N	2.40	0.49
1:A:168:ARG:O	1:A:169:THR:C	2.56	0.49
1:A:109:ASP:C	1:A:109:ASP:OD1	2.54	0.49
1:A:282:ILE:O	1:A:283:PRO:C	2.52	0.49
1:A:147:LEU:C	1:A:148:ARG:O	2.49	0.49
1:A:258:GLU:O	1:A:259:GLU:HB3	2.13	0.49
1:A:210:GLN:NE2	1:A:247:MET:SD	2.86	0.49
1:A:258:GLU:O	1:A:258:GLU:HG2	2.12	0.49
1:A:81:MET:SD	1:A:99:PRO:HG2	2.54	0.48
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.30	0.48
1:A:220:SER:C	1:A:220:SER:N	2.58	0.48
1:A:61:VAL:HA	4:A:338:HOH:O	2.13	0.48
1:A:250:GLU:O	1:A:251:SER:O	2.32	0.48
1:A:96:VAL:C	1:A:98:PHE:H	2.21	0.48
1:A:226:ILE:HG13	1:A:226:ILE:H	1.41	0.48
1:A:131:LEU:CD1	1:A:171:ARG:HG2	2.43	0.48
1:A:208:VAL:O	1:A:212:LEU:HB2	2.14	0.48
1:A:242:THR:HG21	1:A:257:HIS:CG	2.48	0.48
1:A:81:MET:HE1	1:A:84:ARG:HA	1.93	0.48
1:A:3:ASN:O	1:A:94:TRP:CE3	2.67	0.48
1:A:92:PRO:HG3	1:A:94:TRP:CE2	2.49	0.47
1:A:183:GLU:OE1	1:A:184:GLN:HG2	2.14	0.47
1:A:115:ASN:C	1:A:115:ASN:HD22	2.21	0.47
1:A:131:LEU:HD12	1:A:189:GLU:HG3	1.97	0.47
1:A:3:ASN:O	1:A:5:TYR:N	2.45	0.47
1:A:40:ASP:C	1:A:42:LEU:H	2.23	0.47
1:A:195:VAL:O	1:A:196:ALA:CA	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ASN:C	1:A:145:ASN:OD1	2.58	0.47
1:A:23:HIS:CD2	1:A:23:HIS:H	2.31	0.47
1:A:130:MET:O	1:A:238:PHE:HA	2.14	0.47
1:A:170:MET:HE1	1:A:281:SER:HB2	1.97	0.47
1:A:222:VAL:H	1:A:222:VAL:HG23	1.59	0.47
1:A:53:ILE:O	1:A:54:PRO:C	2.57	0.46
1:A:92:PRO:O	1:A:95:LYS:HB2	2.15	0.46
1:A:137:ASN:CG	1:A:222:VAL:HG11	2.40	0.46
1:A:210:GLN:HE21	1:A:247:MET:HE2	1.75	0.46
1:A:217:VAL:HG22	1:A:218:GLY:N	2.29	0.46
1:A:57:PRO:HB2	1:A:85:PHE:CZ	2.51	0.46
1:A:264:GLY:HA3	4:A:349:HOH:O	2.06	0.46
1:A:131:LEU:HD11	1:A:171:ARG:CG	2.46	0.46
1:A:87:MET:O	1:A:88:TYR:C	2.55	0.46
1:A:196:ALA:C	1:A:197:GLY:HA3	2.36	0.46
1:A:206:CYS:SG	1:A:245:VAL:CG1	3.04	0.46
1:A:32:GLY:HA3	1:A:115:ASN:HA	1.96	0.46
1:A:196:ALA:N	1:A:196:ALA:CB	2.76	0.46
1:A:242:THR:CB	1:A:257:HIS:HB2	2.46	0.46
1:A:125:GLU:O	1:A:126:VAL:C	2.56	0.46
1:A:158:ARG:NH1	4:A:316:HOH:O	2.48	0.46
1:A:93:LEU:C	1:A:94:TRP:HA	2.33	0.45
1:A:25:PRO:HG2	1:A:108:VAL:HG23	1.99	0.45
1:A:192:TYR:C	1:A:192:TYR:CD2	2.93	0.45
1:A:281:SER:O	1:A:283:PRO:HD3	2.15	0.45
1:A:42:LEU:HD11	1:A:80:MET:HE3	1.99	0.45
1:A:220:SER:HB2	1:A:221:THR:H	1.82	0.45
1:A:242:THR:HB	1:A:257:HIS:HA	1.97	0.45
1:A:243:ASN:OD1	3:A:293:D1V:H5	2.16	0.45
1:A:260:VAL:CG1	1:A:263:ALA:HB3	2.46	0.45
1:A:92:PRO:HG3	1:A:94:TRP:NE1	2.32	0.45
1:A:284:LEU:CD2	1:A:288:ALA:O	2.56	0.45
1:A:3:ASN:C	1:A:5:TYR:N	2.75	0.45
1:A:109:ASP:HA	1:A:233:LEU:CD2	2.47	0.45
1:A:139:PRO:O	1:A:140:GLY:C	2.60	0.45
1:A:172:GLN:O	1:A:173:ARG:C	2.59	0.45
1:A:222:VAL:N	1:A:223:PRO:CD	2.80	0.45
1:A:135:HIS:NE2	1:A:222:VAL:HG13	2.31	0.45
1:A:178:TRP:CD1	1:A:187:LEU:HB2	2.52	0.44
1:A:168:ARG:HG2	1:A:171:ARG:NH1	2.31	0.44
1:A:229:ARG:NE	4:A:307:HOH:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ILE:CG2	1:A:166:TYR:CE1	3.01	0.44
1:A:166:TYR:CD2	1:A:166:TYR:N	2.84	0.44
1:A:88:TYR:CB	1:A:198:PRO:HB3	2.41	0.44
1:A:188:GLN:H	1:A:188:GLN:HG2	1.53	0.44
1:A:40:ASP:C	1:A:42:LEU:N	2.74	0.44
1:A:206:CYS:SG	1:A:245:VAL:HG11	2.58	0.44
1:A:26:GLN:HE21	1:A:109:ASP:CG	2.26	0.44
1:A:219:MET:CB	1:A:219:MET:O	2.66	0.44
1:A:135:HIS:C	1:A:135:HIS:CD2	2.95	0.43
1:A:160:PRO:HB2	1:A:162:MET:HE2	1.99	0.43
1:A:171:ARG:O	1:A:175:LEU:HB2	2.18	0.43
1:A:254:LYS:HE3	1:A:254:LYS:HB2	1.90	0.43
1:A:84:ARG:HD2	2:A:290:SO4:O2	2.17	0.43
1:A:138:LEU:HA	1:A:138:LEU:HD12	1.40	0.43
1:A:179:LYS:O	1:A:181:MET:N	2.51	0.43
1:A:209:LEU:HD23	1:A:217:VAL:HB	2.01	0.43
1:A:168:ARG:HA	1:A:171:ARG:NH1	2.34	0.43
1:A:176:SER:O	1:A:179:LYS:N	2.46	0.43
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.81	0.43
1:A:92:PRO:HD2	1:A:95:LYS:HD2	2.00	0.43
1:A:137:ASN:ND2	1:A:140:GLY:HA3	2.33	0.43
1:A:223:PRO:CA	1:A:223:PRO:CD	2.93	0.43
1:A:96:VAL:H	1:A:96:VAL:HG23	1.61	0.43
1:A:249:TYR:C	1:A:250:GLU:CG	2.86	0.43
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.61	0.42
1:A:193:VAL:HG13	1:A:217:VAL:HG23	2.01	0.42
1:A:220:SER:HB2	1:A:221:THR:N	2.34	0.42
1:A:221:THR:C	1:A:223:PRO:CD	2.93	0.42
1:A:93:LEU:HB2	1:A:146:PRO:HA	2.01	0.42
1:A:42:LEU:HD23	1:A:42:LEU:HA	1.68	0.42
1:A:92:PRO:CG	1:A:94:TRP:CE2	3.03	0.42
1:A:97:THR:HB	1:A:227:VAL:CG1	2.50	0.41
1:A:148:ARG:CZ	2:A:292:SO4:O1	2.59	0.41
1:A:273:GLN:O	1:A:274:PHE:C	2.63	0.41
1:A:271:LEU:CD2	1:A:275:VAL:HG23	2.48	0.41
1:A:84:ARG:CZ	1:A:220:SER:HB2	2.50	0.41
1:A:104:HIS:O	1:A:106:LEU:N	2.53	0.41
1:A:271:LEU:O	1:A:275:VAL:HG23	2.20	0.41
1:A:39:THR:O	1:A:42:LEU:HB2	2.21	0.41
1:A:277:ILE:O	1:A:278:LEU:C	2.64	0.41
1:A:8:GLU:CD	1:A:8:GLU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLN:HG3	1:A:285:PRO:HG3	2.02	0.41
1:A:38:LEU:C	1:A:38:LEU:CD2	2.90	0.41
1:A:40:ASP:O	1:A:42:LEU:N	2.53	0.41
1:A:57:PRO:HD3	1:A:98:PHE:CD2	2.56	0.41
1:A:147:LEU:N	1:A:147:LEU:CD1	2.60	0.41
1:A:217:VAL:CG2	1:A:218:GLY:N	2.81	0.41
1:A:17:LEU:O	1:A:21:THR:HG22	2.21	0.41
1:A:95:LYS:HA	1:A:98:PHE:HB3	2.02	0.41
1:A:98:PHE:C	1:A:100:VAL:H	2.27	0.41
1:A:99:PRO:O	1:A:102:VAL:N	2.54	0.41
1:A:164:ASP:O	1:A:165:ALA:C	2.61	0.41
1:A:228:ALA:O	1:A:229:ARG:C	2.63	0.41
1:A:113:VAL:O	1:A:113:VAL:CG2	2.69	0.41
1:A:177:THR:O	1:A:178:TRP:C	2.61	0.41
1:A:181:MET:HE2	1:A:183:GLU:HG3	2.02	0.40
1:A:137:ASN:O	1:A:138:LEU:C	2.64	0.40
1:A:253:GLU:OE2	1:A:253:GLU:HA	2.21	0.40

There are no symmetry-related clashes.

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	286/289 (99%)	230 (80%)	35 (12%)	21 (7%)	1 1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	51	SER
1	A	61	VAL
1	A	105	LEU

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	182	GLY
1	A	184	GLN
1	A	221	THR
1	A	251	SER
1	A	259	GLU
1	A	62	PRO
1	A	77	ALA
1	A	104	HIS
1	A	176	SER
1	A	250	GLU
1	A	93	LEU
1	A	172	GLN
1	A	286	ASP
1	A	123	LYS
1	A	54	PRO
1	A	283	PRO

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	239/240 (100%)	177 (74%)	62 (26%)	0 2

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	3	ASN
1	A	8	GLU
1	A	18	LEU
1	A	22	LYS
1	A	26	GLN
1	A	33	SER
1	A	35	LEU
1	A	49	ASP

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Mol	Chain	Res	Type
1	A	52	GLU
1	A	54	PRO
1	A	59	SER
1	A	61	VAL
1	A	67	ARG
1	A	84	ARG
1	A	92	PRO
1	A	98	PHE
1	A	99	PRO
1	A	101	ARG
1	A	102	VAL
1	A	106	LEU
1	A	112	VAL
1	A	115	ASN
1	A	123	LYS
1	A	126	VAL
1	A	131	LEU
1	A	138	LEU
1	A	147	LEU
1	A	148	ARG
1	A	158	ARG
1	A	167	ASP
1	A	172	GLN
1	A	173	ARG
1	A	175	LEU
1	A	180	GLN
1	A	181	MET
1	A	185	ARG
1	A	195	VAL
1	A	208	VAL
1	A	211	LYS
1	A	212	LEU
1	A	221	THR
1	A	227	VAL
1	A	231	CYS
1	A	241	ILE
1	A	245	VAL
1	A	247	MET
1	A	250	GLU
1	A	251	SER
1	A	252	LEU
1	A	253	GLU

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Mol	Chain	Res	Type
1	A	254	LYS
1	A	256	ASN
1	A	258	GLU
1	A	260	VAL
1	A	261	LEU
1	A	266	GLN
1	A	269	GLN
1	A	271	LEU
1	A	273	GLN
1	A	284	LEU
1	A	287	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	115	ASN
1	A	180	GLN
1	A	210	GLN
1	A	243	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are 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	291	-	4,4,4	0.39	0	6,6,6	0.97	0
2	SO4	A	290	-	4,4,4	0.60	0	6,6,6	0.82	0
2	SO4	A	292	-	4,4,4	1.75	1 (25%)	6,6,6	1.24	0
3	D1V	A	293	-	12,13,13	3.15	5 (41%)	16,18,18	4.69	12 (75%)

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
3	D1V	A	293	-	-	-	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	D1V	O4-C3	7.74	1.41	1.23
3	A	293	D1V	C7-C8	4.39	1.46	1.38
3	A	293	D1V	C6-C5	4.24	1.46	1.38
3	A	293	D1V	C4-C1	3.36	1.44	1.40
2	A	292	SO4	O1-S	3.33	1.64	1.44
3	A	293	D1V	C6-C7	2.60	1.44	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	293	D1V	O4-C3-N2	13.54	136.68	120.62
3	A	293	D1V	O4-C3-C4	-8.38	108.31	123.27
3	A	293	D1V	C8-C1-N1	4.49	124.32	118.61
3	A	293	D1V	N2-C2-N1	3.57	130.49	123.63
3	A	293	D1V	C8-C1-C4	-3.40	115.79	119.14
3	A	293	D1V	C5-C4-C3	-3.32	115.26	120.13
3	A	293	D1V	C7-C8-C1	3.15	124.77	118.97
3	A	293	D1V	C5-C4-C1	2.79	122.97	119.78
3	A	293	D1V	C4-C1-N1	-2.51	119.89	122.41
3	A	293	D1V	C1-C4-C3	2.30	121.75	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	293	D1V	C2-N2-C3	-2.23	118.68	123.47
3	A	293	D1V	C6-C7-C8	-2.03	117.74	120.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	290	SO4	2	0
2	A	292	SO4	3	0
3	A	293	D1V	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	146:PRO	C	147:LEU	N	1.91
1	A	198:PRO	C	199:SER	N	1.68
1	A	196:ALA	C	197:GLY	N	1.63
1	A	220:SER	C	221:THR	N	1.20
1	A	223:PRO	C	224:GLU	N	1.18

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, 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	288/289 (99%)	0.64	38 (13%) 7 6	12, 39, 91, 119	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	LEU	11.2
1	A	260	VAL	8.5
1	A	65	ALA	8.3
1	A	254	LYS	6.4
1	A	263	ALA	6.1
1	A	257	HIS	5.7
1	A	287	LYS	5.2
1	A	252	LEU	5.2
1	A	259	GLU	5.2
1	A	258	GLU	5.0
1	A	288	ALA	4.4
1	A	61	VAL	4.4
1	A	62	PRO	4.2
1	A	64	HIS	4.1
1	A	221	THR	4.0
1	A	222	VAL	3.9
1	A	2	GLU	3.7
1	A	251	SER	3.7
1	A	262	ALA	3.7
1	A	220	SER	3.2
1	A	256	ASN	3.1
1	A	223	PRO	3.1
1	A	196	ALA	2.9
1	A	265	LYS	2.8
1	A	66	GLY	2.8
1	A	180	GLN	2.5
1	A	146	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	123	LYS	2.4
1	A	185	ARG	2.4
1	A	255	ALA	2.4
1	A	219	MET	2.3
1	A	249	TYR	2.2
1	A	264	GLY	2.2
1	A	198	PRO	2.2
1	A	289	SER	2.2
1	A	8	GLU	2.1
1	A	248	ASP	2.0
1	A	63	GLY	2.0

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
3	D1V	A	293	12/12	0.87	0.19	36,43,45,49	0
2	SO4	A	291	5/5	0.98	0.05	43,44,46,47	0
2	SO4	A	292	5/5	0.99	0.08	24,31,36,38	0
2	SO4	A	290	5/5	0.99	0.06	24,25,32,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.