



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:01 AM GMT

PDB ID : 3D1V
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

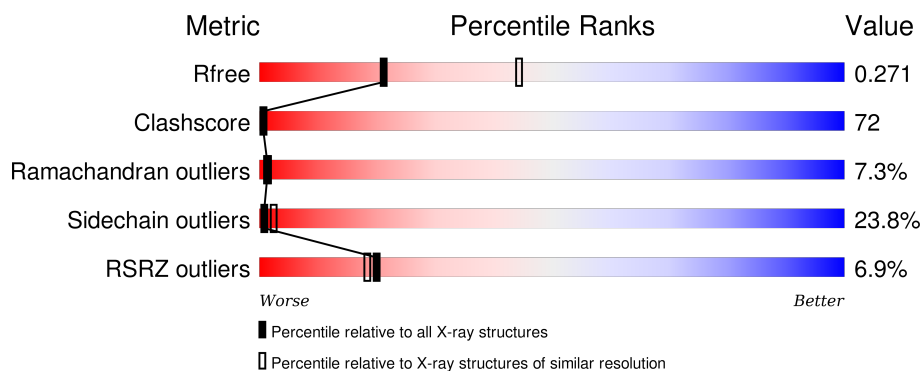
1 Overall quality at a glance

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	-

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:

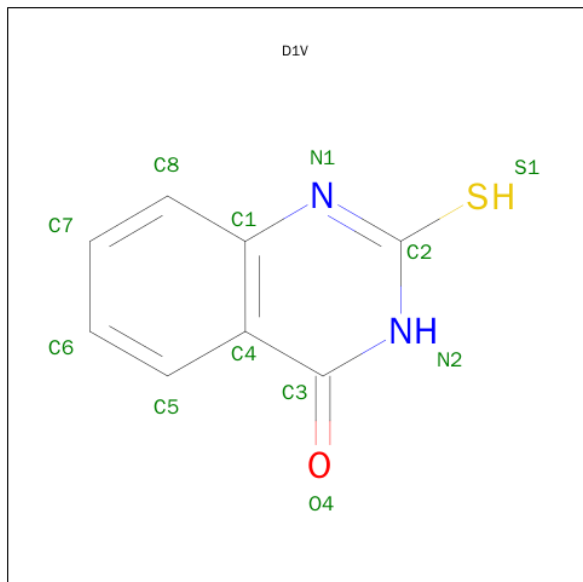
Chain	Residue	Modelled	Actual	Comment	Reference
A	51	SER	GLY	CONFLICT	UNP P00491

- Molecule 2 is SULFATE ION (three-letter code: 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 (three-letter code: D1V) (formula: $C_8H_6N_2OS$).



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

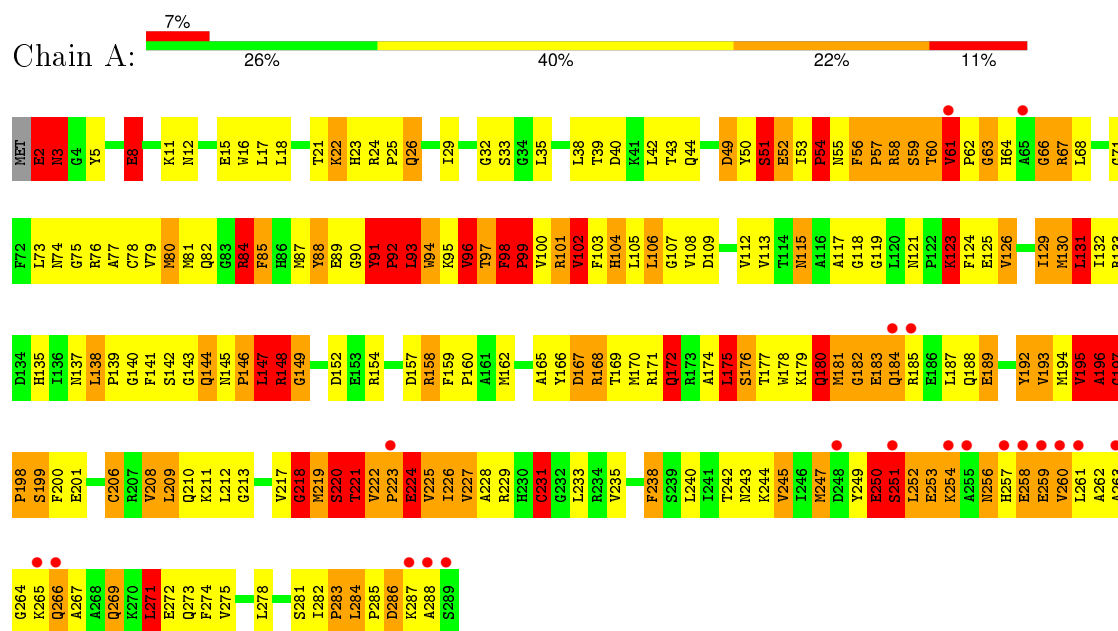
- Molecule 4 is water.

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

3 Residue-property plots

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

• Molecule 1: 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 42.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (42.18-2.70) 98.8 (42.17-2.70)	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 (5.31%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 16192 reflections (0.006%)	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D1V, 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	3.21	124/2303 (5.4%)	2.21	117/3115 (3.8%)

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 (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	PRO	N-CA	41.24	2.17	1.47
1	A	2	GLU	CD-OE1	40.60	1.70	1.25
1	A	221	THR	C-O	36.02	1.91	1.23
1	A	223	PRO	N-CD	33.71	1.95	1.47
1	A	197	GLY	N-CA	32.36	1.94	1.46
1	A	199	SER	CB-OG	27.08	1.77	1.42
1	A	146	PRO	C-N	25.16	1.92	1.34
1	A	221	THR	CB-CG2	22.75	2.27	1.52
1	A	221	THR	CB-OG1	21.34	1.85	1.43
1	A	223	PRO	CA-CB	-19.44	1.14	1.53
1	A	220	SER	C-O	19.41	1.60	1.23
1	A	222	VAL	CB-CG2	-18.06	1.15	1.52
1	A	196	ALA	N-CA	17.48	1.81	1.46
1	A	196	ALA	C-N	16.65	1.63	1.33
1	A	146	PRO	C-O	14.84	1.52	1.23
1	A	198	PRO	C-N	14.77	1.68	1.34
1	A	148	ARG	CG-CD	13.67	1.86	1.51
1	A	147	LEU	C-O	12.96	1.48	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	TRP	CD2-CE3	11.81	1.58	1.40
1	A	223	PRO	CA-C	11.67	1.76	1.52
1	A	97	THR	C-N	11.41	1.60	1.34
1	A	231	CYS	CB-SG	-11.30	1.63	1.82
1	A	149	GLY	N-CA	11.05	1.62	1.46
1	A	2	GLU	CB-CG	11.01	1.73	1.52
1	A	198	PRO	CA-C	10.89	1.74	1.52
1	A	94	TRP	N-CA	10.85	1.68	1.46
1	A	2	GLU	CD-OE2	10.83	1.37	1.25
1	A	92	PRO	N-CD	10.51	1.62	1.47
1	A	225	VAL	N-CA	10.24	1.66	1.46
1	A	220	SER	CA-C	10.15	1.79	1.52
1	A	222	VAL	CA-CB	-10.09	1.33	1.54
1	A	94	TRP	CZ3-CH2	9.76	1.55	1.40
1	A	98	PHE	CD2-CE2	9.69	1.58	1.39
1	A	220	SER	CB-OG	9.68	1.54	1.42
1	A	224	GLU	N-CA	9.63	1.65	1.46
1	A	98	PHE	CG-CD1	-9.57	1.24	1.38
1	A	219	MET	CA-CB	9.53	1.75	1.53
1	A	225	VAL	C-O	9.41	1.41	1.23
1	A	98	PHE	CB-CG	-9.13	1.35	1.51
1	A	198	PRO	N-CD	9.05	1.60	1.47
1	A	196	ALA	CA-CB	8.92	1.71	1.52
1	A	91	TYR	CA-CB	8.92	1.73	1.53
1	A	195	VAL	C-N	8.88	1.54	1.34
1	A	147	LEU	N-CA	-8.81	1.28	1.46
1	A	97	THR	C-O	8.65	1.39	1.23
1	A	195	VAL	C-O	8.60	1.39	1.23
1	A	149	GLY	C-O	8.53	1.37	1.23
1	A	148	ARG	CZ-NH2	8.40	1.44	1.33
1	A	94	TRP	CG-CD1	8.38	1.48	1.36
1	A	97	THR	CB-OG1	8.36	1.59	1.43
1	A	78	CYS	CB-SG	-8.21	1.68	1.82
1	A	147	LEU	CG-CD2	8.10	1.81	1.51
1	A	98	PHE	CG-CD2	-7.99	1.26	1.38
1	A	93	LEU	C-O	7.76	1.38	1.23
1	A	97	THR	CB-CG2	7.65	1.77	1.52
1	A	159	PHE	CD1-CE1	7.65	1.54	1.39
1	A	197	GLY	CA-C	-7.50	1.39	1.51
1	A	98	PHE	CD1-CE1	7.49	1.54	1.39
1	A	218	GLY	C-N	7.41	1.51	1.34
1	A	2	GLU	CG-CD	7.30	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	219	MET	CG-SD	-7.23	1.62	1.81
1	A	146	PRO	N-CA	7.18	1.59	1.47
1	A	8	GLU	CD-OE2	7.09	1.33	1.25
1	A	55	ASN	N-CA	7.08	1.60	1.46
1	A	102	VAL	CB-CG2	-7.06	1.38	1.52
1	A	93	LEU	CB-CG	6.98	1.72	1.52
1	A	61	VAL	N-CA	6.89	1.60	1.46
1	A	222	VAL	C-O	6.89	1.36	1.23
1	A	123	LYS	CD-CE	6.73	1.68	1.51
1	A	193	VAL	CB-CG2	-6.73	1.38	1.52
1	A	144	GLN	CB-CG	-6.72	1.34	1.52
1	A	227	VAL	CB-CG2	-6.66	1.38	1.52
1	A	223	PRO	C-N	-6.63	1.18	1.34
1	A	88	TYR	CD1-CE1	-6.61	1.29	1.39
1	A	129	ILE	CA-CB	-6.36	1.40	1.54
1	A	91	TYR	CE1-CZ	6.33	1.46	1.38
1	A	141	PHE	C-O	6.31	1.35	1.23
1	A	91	TYR	CE2-CZ	6.29	1.46	1.38
1	A	117	ALA	CA-CB	-6.24	1.39	1.52
1	A	2	GLU	N-CA	6.21	1.58	1.46
1	A	8	GLU	CD-OE1	6.17	1.32	1.25
1	A	226	ILE	CB-CG1	6.17	1.71	1.54
1	A	168	ARG	CG-CD	6.11	1.67	1.51
1	A	92	PRO	C-O	6.10	1.35	1.23
1	A	91	TYR	C-O	6.06	1.34	1.23
1	A	223	PRO	C-O	6.03	1.35	1.23
1	A	223	PRO	CB-CG	6.02	1.80	1.50
1	A	220	SER	C-N	-5.97	1.20	1.34
1	A	16	TRP	CB-CG	-5.96	1.39	1.50
1	A	219	MET	C-O	-5.93	1.12	1.23
1	A	92	PRO	N-CA	-5.90	1.37	1.47
1	A	98	PHE	CA-CB	5.89	1.67	1.53
1	A	192	TYR	CB-CG	-5.88	1.42	1.51
1	A	219	MET	C-N	-5.87	1.20	1.34
1	A	192	TYR	CA-CB	-5.82	1.41	1.53
1	A	66	GLY	N-CA	5.79	1.54	1.46
1	A	92	PRO	CG-CD	5.77	1.69	1.50
1	A	238	PHE	CD1-CE1	-5.75	1.27	1.39
1	A	226	ILE	N-CA	5.71	1.57	1.46
1	A	91	TYR	CB-CG	-5.70	1.43	1.51
1	A	85	PHE	CD1-CE1	-5.70	1.27	1.39
1	A	94	TRP	CG-CD2	5.68	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	ARG	CZ-NH1	-5.67	1.25	1.33
1	A	94	TRP	C-O	5.66	1.34	1.23
1	A	224	GLU	CD-OE1	5.63	1.31	1.25
1	A	221	THR	CA-CB	-5.62	1.38	1.53
1	A	98	PHE	N-CA	-5.56	1.35	1.46
1	A	224	GLU	C-O	5.48	1.33	1.23
1	A	219	MET	N-CA	5.46	1.57	1.46
1	A	99	PRO	CB-CG	5.40	1.76	1.50
1	A	101	ARG	CB-CG	-5.39	1.38	1.52
1	A	96	VAL	CB-CG2	-5.38	1.41	1.52
1	A	51	SER	CB-OG	5.30	1.49	1.42
1	A	8	GLU	CG-CD	5.28	1.59	1.51
1	A	195	VAL	CA-CB	-5.22	1.43	1.54
1	A	146	PRO	CA-C	5.21	1.63	1.52
1	A	2	GLU	CA-C	5.20	1.66	1.52
1	A	54	PRO	C-O	5.16	1.33	1.23
1	A	91	TYR	CG-CD1	-5.08	1.32	1.39
1	A	93	LEU	CA-C	-5.07	1.39	1.52
1	A	198	PRO	N-CA	-5.05	1.38	1.47
1	A	172	GLN	CG-CD	5.05	1.62	1.51
1	A	8	GLU	CB-CG	5.04	1.61	1.52
1	A	57	PRO	C-O	-5.03	1.13	1.23

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ARG	NE-CZ-NH2	22.19	131.40	120.30
1	A	223	PRO	N-CD-CG	-19.81	73.48	103.20
1	A	221	THR	CA-CB-OG1	-18.48	70.19	109.00
1	A	196	ALA	C-N-CA	-17.66	85.22	122.30
1	A	221	THR	N-CA-C	14.88	151.19	111.00
1	A	223	PRO	CA-N-CD	-14.83	90.74	111.50
1	A	219	MET	CG-SD-CE	12.34	119.94	100.20
1	A	219	MET	O-C-N	-11.67	104.03	122.70
1	A	222	VAL	CA-CB-CG2	-11.64	93.44	110.90
1	A	80	MET	CG-SD-CE	-11.61	81.63	100.20
1	A	147	LEU	CB-CG-CD2	11.53	130.60	111.00
1	A	97	THR	CA-CB-OG1	-11.19	85.49	109.00
1	A	54	PRO	C-N-CA	-10.95	94.33	121.70
1	A	2	GLU	CG-CD-OE1	-10.71	96.88	118.30
1	A	198	PRO	O-C-N	-10.36	106.13	122.70
1	A	222	VAL	CB-CA-C	-9.98	92.43	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	GLU	CG-CD-OE2	9.93	138.17	118.30
1	A	118	GLY	N-CA-C	-9.71	88.81	113.10
1	A	219	MET	C-N-CA	9.55	145.57	121.70
1	A	199	SER	CB-CA-C	9.52	128.19	110.10
1	A	91	TYR	C-N-CD	9.47	148.29	128.40
1	A	93	LEU	C-N-CA	-9.04	99.10	121.70
1	A	195	VAL	CA-C-O	8.99	138.99	120.10
1	A	101	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	A	93	LEU	CB-CA-C	8.49	126.33	110.20
1	A	98	PHE	CB-CA-C	8.40	127.20	110.40
1	A	223	PRO	N-CA-CB	-8.31	93.33	103.30
1	A	227	VAL	CB-CA-C	8.21	127.00	111.40
1	A	146	PRO	CA-C-O	8.18	139.84	120.20
1	A	91	TYR	CB-CG-CD2	8.17	125.90	121.00
1	A	219	MET	CA-C-N	8.02	134.83	117.20
1	A	198	PRO	CA-C-N	8.01	134.83	117.20
1	A	92	PRO	N-CA-C	7.96	132.81	112.10
1	A	219	MET	N-CA-CB	7.84	124.72	110.60
1	A	148	ARG	CA-C-N	7.82	131.84	116.20
1	A	206	CYS	CA-CB-SG	-7.77	100.01	114.00
1	A	199	SER	CA-CB-OG	-7.76	90.24	111.20
1	A	175	LEU	CA-CB-CG	7.74	133.10	115.30
1	A	54	PRO	O-C-N	-7.74	110.32	122.70
1	A	94	TRP	CD1-CG-CD2	-7.59	100.23	106.30
1	A	131	LEU	CA-CB-CG	7.55	132.67	115.30
1	A	92	PRO	N-CD-CG	-7.52	91.92	103.20
1	A	61	VAL	N-CA-C	7.42	131.03	111.00
1	A	93	LEU	CB-CG-CD1	-7.42	98.39	111.00
1	A	200	PHE	N-CA-CB	-7.41	97.26	110.60
1	A	224	GLU	CB-CA-C	7.31	125.01	110.40
1	A	225	VAL	CG1-CB-CG2	-7.30	99.22	110.90
1	A	88	TYR	CB-CG-CD1	-7.26	116.64	121.00
1	A	148	ARG	NH1-CZ-NH2	-7.25	111.42	119.40
1	A	91	TYR	CB-CG-CD1	-7.22	116.67	121.00
1	A	146	PRO	O-C-N	-7.21	111.16	122.70
1	A	75	GLY	N-CA-C	-7.14	95.25	113.10
1	A	91	TYR	CZ-CE2-CD2	-7.09	113.42	119.80
1	A	98	PHE	CA-C-O	-7.08	105.22	120.10
1	A	196	ALA	CA-C-O	7.00	134.81	120.10
1	A	91	TYR	CG-CD2-CE2	6.99	126.89	121.30
1	A	148	ARG	CA-C-O	-6.93	105.55	120.10
1	A	92	PRO	CA-CB-CG	-6.89	90.90	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	97	THR	N-CA-C	-6.83	92.56	111.00
1	A	196	ALA	O-C-N	-6.74	111.75	123.20
1	A	219	MET	CB-CA-C	-6.72	96.97	110.40
1	A	58	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	88	TYR	CB-CG-CD2	6.69	125.01	121.00
1	A	51	SER	N-CA-CB	-6.60	100.60	110.50
1	A	195	VAL	C-N-CA	-6.56	105.31	121.70
1	A	226	ILE	CA-CB-CG1	-6.53	98.59	111.00
1	A	97	THR	CB-CA-C	6.51	129.17	111.60
1	A	192	TYR	N-CA-CB	-6.49	98.92	110.60
1	A	222	VAL	O-C-N	-6.40	108.94	121.10
1	A	91	TYR	CA-C-O	-6.35	106.77	120.10
1	A	148	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	A	220	SER	C-N-CA	-6.27	106.03	121.70
1	A	221	THR	N-CA-CB	-6.25	98.43	110.30
1	A	148	ARG	CB-CG-CD	6.16	127.61	111.60
1	A	148	ARG	CD-NE-CZ	-6.14	115.00	123.60
1	A	59	SER	CB-CA-C	-6.13	98.45	110.10
1	A	195	VAL	CG1-CB-CG2	6.11	120.68	110.90
1	A	218	GLY	C-N-CA	-6.02	106.65	121.70
1	A	101	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	131	LEU	CB-CG-CD2	5.96	121.12	111.00
1	A	147	LEU	C-N-CA	-5.95	106.82	121.70
1	A	90	GLY	C-N-CA	-5.92	106.90	121.70
1	A	2	GLU	N-CA-C	5.87	126.84	111.00
1	A	99	PRO	CB-CG-CD	-5.75	84.08	106.50
1	A	91	TYR	N-CA-CB	-5.69	100.36	110.60
1	A	92	PRO	CA-C-O	-5.63	106.69	120.20
1	A	91	TYR	C-N-CA	-5.63	98.36	122.00
1	A	223	PRO	CA-C-O	-5.62	106.70	120.20
1	A	195	VAL	O-C-N	-5.58	113.78	122.70
1	A	98	PHE	CG-CD1-CE1	5.56	126.92	120.80
1	A	148	ARG	C-N-CA	5.52	133.89	122.30
1	A	91	TYR	CB-CA-C	-5.50	99.40	110.40
1	A	143	GLY	CA-C-O	5.49	130.48	120.60
1	A	219	MET	CB-CG-SD	5.45	128.75	112.40
1	A	224	GLU	N-CA-CB	-5.45	100.79	110.60
1	A	231	CYS	CB-CA-C	-5.44	99.52	110.40
1	A	199	SER	N-CA-C	-5.44	96.32	111.00
1	A	221	THR	OG1-CB-CG2	-5.42	97.53	110.00
1	A	98	PHE	N-CA-C	-5.39	96.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	224	GLU	CG-CD-OE1	-5.35	107.59	118.30
1	A	97	THR	C-N-CA	-5.27	108.53	121.70
1	A	147	LEU	CB-CA-C	-5.27	100.19	110.20
1	A	93	LEU	CD1-CG-CD2	5.20	126.09	110.50
1	A	98	PHE	CE1-CZ-CE2	-5.20	110.65	120.00
1	A	271	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	A	89	GLU	C-N-CA	-5.17	111.45	122.30
1	A	63	GLY	N-CA-C	-5.15	100.23	113.10
1	A	94	TRP	O-C-N	5.10	130.86	122.70
1	A	142	SER	N-CA-C	5.10	124.77	111.00
1	A	222	VAL	N-CA-C	-5.08	97.28	111.00
1	A	225	VAL	CA-C-O	-5.06	109.47	120.10
1	A	224	GLU	OE1-CD-OE2	5.05	129.36	123.30
1	A	130	MET	CG-SD-CE	-5.05	92.12	100.20
1	A	218	GLY	CA-C-O	5.02	129.64	120.60
1	A	221	THR	CA-C-N	-5.01	106.19	117.20

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	Mainchain,Peptide
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	324	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	324	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 72.

All (324) 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:147:LEU:CG	1:A:147:LEU:CD2	1.81	1.57
1:A:223:PRO:CG	1:A:223:PRO:CB	1.80	1.57
1:A:97:THR:CB	1:A:97:THR:CG2	1.77	1.56
1:A:198:PRO:C	1:A:198:PRO:CA	1.74	1.54
1:A:148:ARG:CD	1:A:148:ARG:CG	1.86	1.54
1:A:219:MET:CB	1:A:219:MET:CA	1.74	1.54
1:A:99:PRO:CB	1:A:99:PRO:CG	1.77	1.53
1:A:223:PRO:CA	1:A:223:PRO:C	1.76	1.52
1:A:94:TRP:CA	1:A:94:TRP:N	1.68	1.50
1:A:220:SER:CA	1:A:220:SER:C	1.79	1.49
1:A:198:PRO:C	1:A:199:SER:N	1.68	1.45
1:A:196:ALA:CA	1:A:196:ALA:N	1.81	1.42
1:A:199:SER:OG	1:A:199:SER:CB	1.77	1.32
1:A:197:GLY:N	1:A:197:GLY:CA	1.94	1.30
1:A:223:PRO:N	1:A:223:PRO:CD	1.95	1.28
1:A:2:GLU:OE1	1:A:2:GLU:CD	1.70	1.28
1:A:22:LYS:HA	1:A:22:LYS:CE	1.61	1.28
1:A:146:PRO:C	1:A:147:LEU:N	1.91	1.23
1:A:148:ARG:NH1	2:A:292:SO4:O1	1.79	1.16
1:A:146:PRO:HG3	1:A:223:PRO:HA	1.19	1.13
1:A:221:THR:CG2	1:A:221:THR:CB	2.27	1.11
1:A:243:ASN:HD21	1:A:256:ASN:HA	0.98	1.10
1:A:243:ASN:ND2	1:A:256:ASN:HA	1.65	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:LEU:HD22	1:A:71:GLY:HA3	1.14	1.10
1:A:223:PRO:N	1:A:223:PRO:CG	2.16	1.08
1:A:221:THR:C	1:A:221:THR:O	1.91	1.08
1:A:22:LYS:HE3	1:A:22:LYS:HA	1.15	1.08
1:A:223:PRO:N	1:A:223:PRO:CA	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	0.97
1:A:147:LEU:HD22	1:A:226:ILE:HG22	1.49	0.95
1:A:22:LYS:CE	1:A:22:LYS:CA	2.47	0.92
1:A:22:LYS:HE3	1:A:22:LYS:CA	2.00	0.91
1:A:223:PRO:CA	1:A:223:PRO:CG	2.49	0.90
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:HE2	1:A:22:LYS:HA	1.51	0.89
1:A:223:PRO:O	1:A:227:VAL:HG13	1.72	0.89
1:A:201:GLU:OE1	3:A:293:D1V:S1	2.30	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:223:PRO:CB	1:A:223:PRO:C	2.41	0.88
1:A:97:THR:HG21	1:A:146:PRO:HB3	1.54	0.87
1:A:196:ALA:C	1:A:197:GLY:CA	2.43	0.86
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:201:GLU:CD	3:A:293:D1V:S1	2.55	0.85
1:A:147:LEU:HG	1:A:147:LEU:CD2	2.04	0.83
1:A:201:GLU:CD	3:A:293:D1V:HS1	1.80	0.83
1:A:196:ALA:O	1:A:197:GLY:O	1.96	0.82
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:247:MET:HE3	1:A:247:MET:HA	1.62	0.80
1:A:179:LYS:O	1:A:182:GLY:N	2.10	0.79
1:A:97:THR:CG2	1:A:97:THR:CA	2.59	0.78
1:A:222:VAL:O	1:A:226:ILE:HG13	1.83	0.77
1:A:199:SER:CA	1:A:199:SER:OG	2.32	0.77
1:A:201:GLU:N	1:A:201:GLU:OE1	2.15	0.77
1:A:42:LEU:CD2	1:A:71:GLY:HA3	2.06	0.77
1:A:219:MET:C	1:A:219:MET:CB	2.54	0.77
1:A:81:MET:CE	1:A:84:ARG:HA	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TRP:C	1:A:94:TRP:N	2.39	0.75
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:CG	1:A:219:MET:CA	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:220:SER:C	1:A:220:SER:CB	2.55	0.73
1:A:220:SER:CA	1:A:221:THR:N	2.51	0.73
1:A:223:PRO:N	1:A:223:PRO:CB	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:146:PRO:HG2	1:A:226:ILE:HB	1.72	0.71
1:A:60:THR:O	1:A:61:VAL:HB	1.90	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
1:A:93:LEU:O	1:A:94:TRP:CA	2.39	0.71
1:A:94:TRP:N	1:A:95:LYS:H	1.89	0.70
1:A:49:ASP:O	1:A:52:GLU:HG3	1.91	0.70
1:A:201:GLU:OE2	3:A:293:D1V: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: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:198:PRO:CB	1:A:198:PRO:C	2.62	0.66
1:A:81:MET:HE1	1:A:84:ARG:HA	1.77	0.66
1:A:265:LYS:O	1:A:269:GLN:CG	2.44	0.66
1:A:196:ALA:C	1:A:196:ALA:N	2.49	0.66
1:A:38:LEU:C	1:A:38:LEU:HD23	2.16	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:249:TYR:C	1:A:250:GLU:HG3	2.16	0.65
1:A:121:ASN:O	1:A:124:PHE:HB2	1.97	0.65
1:A:104:HIS:O	1:A:107:GLY:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:ARG:CG	1:A:171:ARG:HH21	2.10	0.64
1:A:113:VAL:HG21	1:A:221:THR:CG2	2.27	0.64
1:A:177:THR:HA	1:A:180:GLN:CG	2.28	0.63
1:A:109:ASP:HA	1:A:233:LEU:HD22	1.81	0.63
1:A:29:ILE:HB	1:A:80:MET:HG2	1.79	0.63
1:A:252:LEU:HD12	1:A:252:LEU:H	1.62	0.63
1:A:252:LEU:CD1	1:A:252:LEU:H	2.11	0.63
1:A:195:VAL:C	1:A:196:ALA:CA	2.67	0.63
1:A:147:LEU:CD1	1:A:147:LEU:CD2	2.71	0.62
1:A:147:LEU:CD2	1:A:226:ILE:HG22	2.27	0.62
1:A:49:ASP:HB3	1:A:51:SER:CB	2.29	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:247:MET:CE	1:A:247:MET:HA	2.29	0.61
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:210:GLN:HE21	1:A:247:MET:CE	2.13	0.61
1:A:76:ARG:NH2	1:A:282:ILE:O	2.32	0.61
1:A:223:PRO:HB2	1:A:223:PRO:C	2.22	0.60
1:A:210:GLN:NE2	1:A:247:MET:CE	2.64	0.60
1:A:97:THR:HG21	1:A:146:PRO:CB	2.30	0.60
1:A:97:THR:CG2	1:A:223:PRO:HB3	2.31	0.60
1:A:168:ARG:HG2	1:A:171:ARG:HH12	1.67	0.60
1:A:74:ASN:CG	1:A:74:ASN:O	2.37	0.60
1:A:91:TYR:HB3	1:A:95:LYS:HB2	1.84	0.59
1:A:113:VAL:O	1:A:113:VAL:HG23	2.02	0.59
1:A:92:PRO:C	1:A:94:TRP:N	2.51	0.59
1:A:146:PRO:C	1:A:147:LEU:CA	2.70	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:265:LYS:O	1:A:269:GLN:HG3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:222:VAL:HG12	1:A:226:ILE:HD11	1.87	0.56
1:A:198:PRO:C	1:A:199:SER:O	2.44	0.56
1:A:129:ILE:CG2	1:A:130:MET:N	2.68	0.56
1:A:38:LEU:HD22	1:A:80:MET:SD	2.46	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:CE2	2.89	0.56
1:A:187:LEU:CD1	1:A:274:PHE:HE2	2.19	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: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:67:ARG:NE	1:A:82:GLN:OE1	2.37	0.55
1:A:81:MET:HE2	1:A:84:ARG:HA	1.88	0.55
1:A:84:ARG:NE	1:A:220:SER:HB2	2.22	0.55
1:A:177:THR:CA	1:A:180:GLN:HG2	2.36	0.55
1:A:149:GLY:O	1:A:158:ARG:NH2	2.31	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:79:VAL:O	1:A:79:VAL:CG1	2.55	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:92:PRO:C	1:A:94:TRP:H	2.11	0.54
1:A:256:ASN:H	1:A:259:GLU:CD	2.11	0.54
1:A:63:GLY:O	1:A:66:GLY:N	2.40	0.54
1:A:43:THR:O	1:A:44:GLN:HB2	2.07	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: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:O	1:A:198:PRO:CA	2.51	0.53
1:A:252:LEU:N	1:A:252:LEU:HD12	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:222:VAL:HG12	1:A:222:VAL:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TYR:O	1:A:250:GLU:CG	2.46	0.51
1:A:22:LYS:HE2	1:A:22:LYS:CA	2.29	0.51
1:A:262:ALA:O	1:A:266:GLN:CB	2.59	0.51
1:A:250:GLU:OE2	1:A:253:GLU:HG2	2.10	0.51
1:A:98:PHE:C	1:A:100:VAL:N	2.61	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:197:GLY:C	1:A:197:GLY:N	2.61	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:201:GLU:N	1:A:201:GLU:CD	2.64	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:96:VAL:C	1:A:98:PHE:N	2.64	0.50
1:A:97:THR:HB	1:A:97:THR:CG2	2.20	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:56:PHE:O	1:A:57:PRO:C	2.47	0.49
1:A:220:SER:O	1:A:222:VAL:N	2.40	0.49
1:A:198:PRO:O	1:A:199:SER:N	2.39	0.49
1:A:258:GLU:O	1:A:259:GLU:HB3	2.13	0.49
1:A:258:GLU:HG2	1:A:258:GLU:O	2.12	0.49
1:A:210:GLN:NE2	1:A:247:MET:SD	2.86	0.49
1:A:63:GLY:C	1:A:66:GLY:H	2.16	0.49
1:A:3:ASN:C	1:A:5:TYR:H	2.16	0.48
1:A:147:LEU:HA	1:A:147:LEU:HD12	1.30	0.48
1:A:81:MET:SD	1:A:99:PRO:HG2	2.54	0.48
1:A:250:GLU:O	1:A:251:SER:O	2.32	0.48
1:A:61:VAL:HA	4:A:338:HOH:O	2.13	0.48
1:A:160:PRO:HB2	1:A:162:MET:HE2	1.95	0.48
1:A:221:THR:O	1:A:222:VAL:C	2.52	0.48
1:A:226:ILE:H	1:A:226:ILE:HG13	1.41	0.48
1:A:131:LEU:CD1	1:A:171:ARG:HG2	2.43	0.48
1:A:242:THR:HG21	1:A:257:HIS:CG	2.48	0.48
1:A:208:VAL:O	1:A:212:LEU:HB2	2.14	0.48
1:A:210:GLN:HE21	1:A:247:MET:HE1	1.78	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:103:PHE:O	1:A:104:HIS:C	2.53	0.47
1:A:183:GLU:OE1	1:A:184:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LEU:HD12	1:A:189:GLU:HG3	1.97	0.47
1:A:99:PRO:O	1:A:100:VAL:C	2.49	0.47
1:A:3:ASN:O	1:A:5:TYR:N	2.45	0.47
1:A:195:VAL:O	1:A:196:ALA:CA	2.63	0.47
1:A:222:VAL:HG23	1:A:222:VAL:H	1.59	0.47
1:A:130:MET:O	1:A:238:PHE:HA	2.14	0.47
1:A:23:HIS:H	1:A:23:HIS:CD2	2.31	0.47
1:A:92:PRO:O	1:A:95:LYS:HB2	2.15	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:11:LYS:O	1:A:12:ASN:C	2.52	0.46
1:A:206:CYS:SG	1:A:245:VAL:CG1	3.04	0.46
1:A:8:GLU:H	1:A:8:GLU:CD	2.19	0.46
1:A:196:ALA:CB	1:A:196:ALA:N	2.76	0.46
1:A:242:THR:CB	1:A:257:HIS:HB2	2.46	0.46
1:A:32:GLY:HA3	1:A:115:ASN:HA	1.96	0.46
1:A:282:ILE:O	1:A:283:PRO:C	2.52	0.46
1:A:158:ARG:NH1	4:A:316:HOH:O	2.48	0.46
1:A:25:PRO:HG2	1:A:108:VAL:HG23	1.99	0.45
1:A:220:SER:N	1:A:220:SER:C	2.58	0.45
1:A:281:SER:O	1:A:283:PRO:HD3	2.15	0.45
1:A:146:PRO:C	1:A:147:LEU:HD13	2.37	0.45
1:A:220:SER:HB2	1:A:221:THR:H	1.82	0.45
1:A:243:ASN:OD1	3:A:293:D1V:H5	2.16	0.45
1:A:109:ASP:OD1	1:A:109:ASP:C	2.54	0.45
1:A:242:THR:HB	1:A:257:HIS:HA	1.97	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:109:ASP:HA	1:A:233:LEU:CD2	2.47	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:168:ARG:O	1:A:169:THR:C	2.56	0.44
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
1:A:166:TYR:CD2	1:A:166:TYR:N	2.84	0.44
1:A:132:ILE:CG2	1:A:166:TYR:CE1	3.01	0.44
1:A:88:TYR:CB	1:A:198:PRO:HB3	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLN:HG2	1:A:188:GLN:H	1.53	0.44
1:A:147:LEU:C	1:A:148:ARG:O	2.49	0.44
1:A:206:CYS:SG	1:A:245:VAL:HG11	2.58	0.44
1:A:219:MET:O	1:A:219:MET:CB	2.66	0.44
1:A:96:VAL:C	1:A:98:PHE:H	2.21	0.43
1:A:171:ARG:O	1:A:175:LEU:HB2	2.18	0.43
1:A:254:LYS:HB2	1:A:254:LYS:HE3	1.90	0.43
1:A:217:VAL:CG2	1:A:218:GLY:N	2.81	0.43
1:A:84:ARG:HD2	2:A:290:SO4:O2	2.17	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:138:LEU:HA	1:A:138:LEU:HD12	1.40	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:92:PRO:HD2	1:A:95:LYS:HD2	2.00	0.43
1:A:196:ALA:C	1:A:197:GLY:HA3	2.36	0.43
1:A:68:LEU:HA	1:A:68:LEU:HD12	1.81	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:106:LEU:HD12	1:A:106:LEU:HA	1.61	0.42
1:A:220:SER:HB2	1:A:221:THR:N	2.34	0.42
1:A:87:MET:O	1:A:88:TYR:C	2.55	0.42
1:A:193:VAL:HG13	1:A:217:VAL:HG23	2.01	0.42
1:A:249:TYR:C	1:A:250:GLU:CG	2.86	0.42
1:A:40:ASP:C	1:A:42:LEU:H	2.23	0.42
1:A:115:ASN:C	1:A:115:ASN:HD22	2.21	0.42
1:A:93:LEU:HB2	1:A:146:PRO:HA	2.01	0.42
1:A:145:ASN:OD1	1:A:145:ASN:C	2.58	0.42
1:A:53:ILE:O	1:A:54:PRO:C	2.57	0.42
1:A:92:PRO:CG	1:A:94:TRP:CE2	3.03	0.42
1:A:42:LEU:HA	1:A:42:LEU:HD23	1.68	0.42
1:A:210:GLN:NE2	1:A:247:MET:HE2	2.33	0.42
1:A:148:ARG:CZ	2:A:292:SO4:O1	2.59	0.41
1:A:97:THR:HB	1:A:227:VAL:CG1	2.50	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:147:LEU:CD1	1:A:147:LEU:N	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:CG	1:A:222:VAL:HG11	2.40	0.41
1:A:57:PRO:HD3	1:A:98:PHE:CD2	2.56	0.41
1:A:40:ASP:O	1:A:42:LEU:N	2.53	0.41
1:A:26:GLN:HG3	1:A:285:PRO:HG3	2.02	0.41
1:A:95:LYS:HA	1:A:98:PHE:HB3	2.02	0.41
1:A:99:PRO:O	1:A:102:VAL:N	2.54	0.41
1:A:40:ASP:C	1:A:42:LEU:N	2.74	0.41
1:A:17:LEU:O	1:A:21:THR:HG22	2.21	0.41
1:A:125:GLU:O	1:A:126:VAL:C	2.56	0.41
1:A:192:TYR:CD2	1:A:192:TYR:C	2.93	0.41
1:A:113:VAL:CG2	1:A:113:VAL:O	2.69	0.41
1:A:139:PRO:O	1:A:140:GLY:C	2.60	0.41
1:A:3:ASN:C	1:A:5:TYR:N	2.75	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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
1	A	180	GLN
1	A	182	GLY
1	A	184	GLN

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Mol	Chain	Res	Type
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%)	182 (76%)	57 (24%)	1 2

All (57) 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	49	ASP
1	A	52	GLU
1	A	54	PRO
1	A	56	PHE
1	A	59	SER

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Mol	Chain	Res	Type
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	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	221	THR
1	A	231	CYS
1	A	245	VAL
1	A	250	GLU
1	A	251	SER
1	A	252	LEU
1	A	253	GLU
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

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Mol	Chain	Res	Type
1	A	273	GLN
1	A	284	LEU
1	A	287	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) 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
1	A	256	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 carbohydrates 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	290	-	4,4,4	0.82	0	6,6,6	0.94	1 (16%)
2	SO4	A	291	-	4,4,4	0.24	0	6,6,6	1.34	1 (16%)
2	SO4	A	292	-	4,4,4	2.82	1 (25%)	6,6,6	1.67	1 (16%)
3	D1V	A	293	-	12,13,13	3.20	7 (58%)	9,18,18	2.55	5 (55%)

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
2	SO4	A	290	-	-	0/0/0/0	0/0/0/0
2	SO4	A	291	-	-	0/0/0/0	0/0/0/0
2	SO4	A	292	-	-	0/0/0/0	0/0/0/0
3	D1V	A	293	-	-	0/0/0/0	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	D1V	C6-C7	2.31	1.44	1.38
3	A	293	D1V	C2-N2	2.34	1.37	1.34
3	A	293	D1V	C3-N2	3.13	1.38	1.33
3	A	293	D1V	C3-C4	3.31	1.46	1.41
3	A	293	D1V	C6-C5	4.14	1.46	1.36
3	A	293	D1V	C7-C8	4.25	1.46	1.36
2	A	292	SO4	O1-S	5.11	1.64	1.47
3	A	293	D1V	O4-C3	6.97	1.41	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	292	SO4	O2-S-O1	-3.68	97.82	109.50
3	A	293	D1V	C8-C1-C4	-2.56	115.79	120.10
2	A	290	SO4	O4-S-O3	-2.20	100.04	108.98
3	A	293	D1V	C7-C8-C1	2.94	124.77	120.06
2	A	291	SO4	O2-S-O1	2.96	118.86	109.50
3	A	293	D1V	C5-C4-C1	3.27	122.97	117.56
3	A	293	D1V	C3-C4-C1	3.28	121.75	118.54
3	A	293	D1V	C8-C1-N1	3.52	124.32	118.73

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](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/289 (99%)	0.28	20 (6%) 20 18	12, 39, 91, 119	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	GLU	8.1
1	A	258	GLU	7.6
1	A	260	VAL	7.5
1	A	254	LYS	6.2
1	A	65	ALA	5.7
1	A	263	ALA	5.4
1	A	261	LEU	5.2
1	A	255	ALA	5.0
1	A	289	SER	4.3
1	A	288	ALA	3.8
1	A	257	HIS	3.7
1	A	184	GLN	3.4
1	A	185	ARG	2.8
1	A	287	LYS	2.7
1	A	61	VAL	2.5
1	A	266	GLN	2.4
1	A	251	SER	2.2
1	A	223	PRO	2.1
1	A	265	LYS	2.1
1	A	248	ASP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	D1V	A	293	12/12	0.91	0.21	0.26	36,43,45,49	0
2	SO4	A	291	5/5	0.99	0.11	-0.57	43,44,46,47	0
2	SO4	A	290	5/5	0.99	0.14	-0.70	24,25,32,35	0
2	SO4	A	292	5/5	0.97	0.18	-0.71	24,31,36,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.