



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 AM UTC

PDB ID : 1ULA / pdb_00001ula
Title : APPLICATION OF CRYSTALLOGRAPHIC AND MODELING METHODS
IN THE DESIGN OF PURINE NUCLEOSIDE PHOSPHORYLASE IN-
HIBITORS
Authors : Ealick, S.E.; Rule, S.A.; Carter, D.C.; Greenhough, T.J.; Babu, Y.S.; Cook,
W.J.; Habash, J.; Helliwell, J.R.; Stoeckler, J.D.; Parksjunior, R.E.; Chen,
S.-F.; Bugg, C.E.
Deposited on : 1991-11-05
Resolution : 2.75 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)

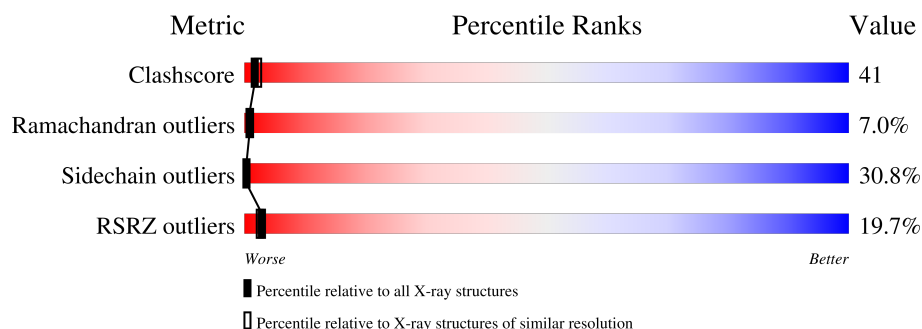
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2268 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
1	A	289	Total	C	N	O	S	0	0	0
			2258	1434	395	413	16			

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

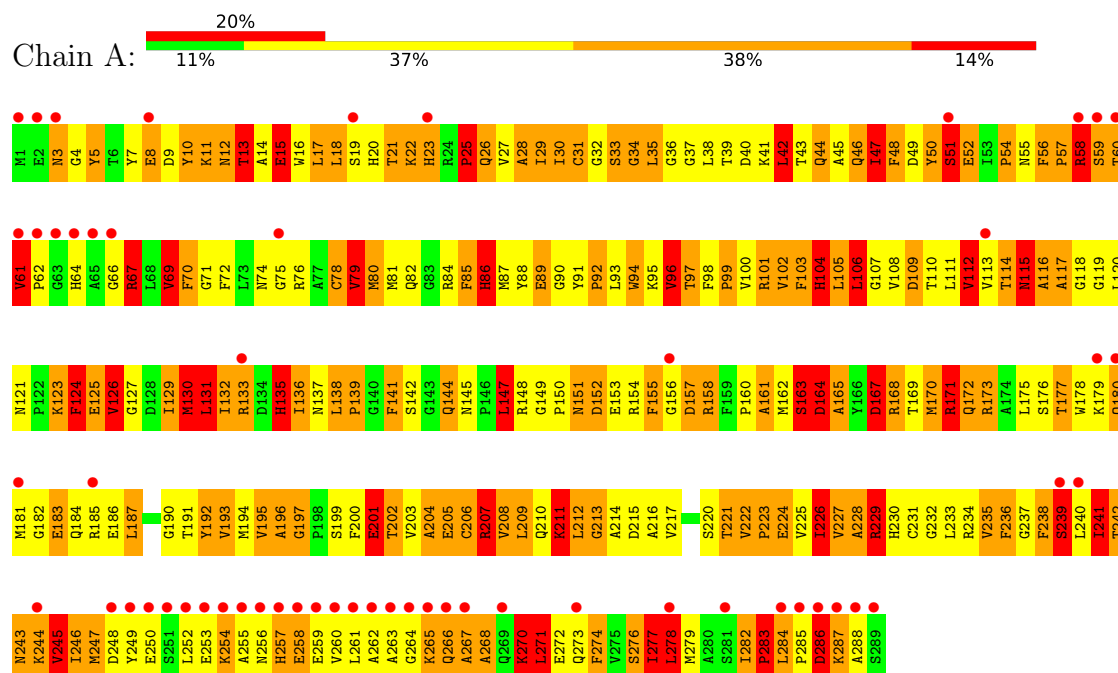


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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	142.90Å 142.90Å 165.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.75 99.05 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.75) 98.0 (99.05-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.76Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.202 , (Not available) 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	2268	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.73	23/2310 (1.0%)	3.19	347/3125 (11.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	ASP	CA-CB	8.37	1.67	1.53
1	A	145	ASN	N-CA	8.32	1.55	1.45
1	A	119	GLY	N-CA	7.88	1.55	1.44
1	A	54	PRO	C-O	7.34	1.33	1.24
1	A	156	GLY	N-CA	7.02	1.52	1.44
1	A	116	ALA	C-N	-6.60	1.25	1.33
1	A	208	VAL	N-CA	6.60	1.54	1.46
1	A	164	ASP	N-CA	-6.55	1.37	1.46
1	A	204	ALA	C-N	-6.41	1.25	1.33
1	A	222	VAL	N-CA	6.14	1.54	1.46
1	A	106	LEU	N-CA	6.13	1.53	1.46
1	A	125	GLU	N-CA	6.06	1.53	1.45
1	A	115	ASN	C-N	-6.03	1.25	1.33
1	A	144	GLN	C-O	5.72	1.29	1.23
1	A	67	ARG	CD-NE	5.67	1.54	1.46
1	A	222	VAL	CA-C	-5.64	1.47	1.52
1	A	163	SER	N-CA	5.55	1.52	1.46
1	A	36	GLY	N-CA	5.29	1.54	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	VAL	C-N	-5.27	1.26	1.33
1	A	91	TYR	CA-CB	5.24	1.63	1.53
1	A	61	VAL	N-CA	-5.13	1.40	1.46
1	A	237	GLY	N-CA	-5.13	1.40	1.45
1	A	282	ILE	CA-CB	5.08	1.59	1.53

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ALA	CA-C-N	15.84	146.74	121.87
1	A	196	ALA	C-N-CA	15.84	146.74	121.87
1	A	154	ARG	NE-CZ-NH2	14.36	132.13	119.20
1	A	141	PHE	CA-CB-CG	13.98	127.78	113.80
1	A	60	THR	CA-C-N	13.30	146.73	122.13
1	A	60	THR	C-N-CA	13.30	146.73	122.13
1	A	168	ARG	CD-NE-CZ	12.13	141.38	124.40
1	A	106	LEU	N-CA-C	-12.03	98.15	111.14
1	A	163	SER	CA-C-N	11.78	144.04	121.54
1	A	163	SER	C-N-CA	11.78	144.04	121.54
1	A	121	ASN	CB-CA-C	11.65	126.43	109.08
1	A	204	ALA	N-CA-C	-11.61	98.15	111.03
1	A	157	ASP	CA-CB-CG	11.56	124.16	112.60
1	A	164	ASP	CA-CB-CG	-11.41	101.19	112.60
1	A	208	VAL	N-CA-C	-11.08	100.08	110.82
1	A	208	VAL	CB-CA-C	11.06	126.53	112.04
1	A	36	GLY	N-CA-C	-11.06	102.50	114.67
1	A	101	ARG	CB-CG-CD	10.96	136.52	111.30
1	A	116	ALA	CA-C-N	10.81	140.10	121.29
1	A	116	ALA	C-N-CA	10.81	140.10	121.29
1	A	12	ASN	OD1-CG-ND2	10.79	133.39	122.60
1	A	245	VAL	CA-C-O	10.63	134.07	120.78
1	A	201	GLU	CA-C-O	-10.62	108.81	120.92
1	A	90	GLY	CA-C-N	10.55	134.81	120.67
1	A	90	GLY	C-N-CA	10.55	134.81	120.67
1	A	3	ASN	CA-CB-CG	-10.53	102.07	112.60
1	A	164	ASP	N-CA-CB	-10.29	93.09	110.49
1	A	104	HIS	CA-CB-CG	10.27	124.07	113.80
1	A	207	ARG	CD-NE-CZ	-10.27	110.03	124.40
1	A	79	VAL	CA-C-O	-10.24	108.68	120.67
1	A	243	ASN	CA-CB-CG	10.22	122.82	112.60
1	A	16	TRP	O-C-N	10.20	132.99	122.08
1	A	124	PHE	CA-CB-CG	10.07	123.87	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	THR	CA-C-O	-9.88	109.95	120.63
1	A	30	ILE	O-C-N	9.75	133.54	123.20
1	A	154	ARG	CA-C-O	9.75	131.37	119.38
1	A	153	GLU	CA-C-O	-9.62	108.25	119.61
1	A	211	LYS	N-CA-CB	9.59	124.22	110.12
1	A	79	VAL	O-C-N	9.44	133.38	123.18
1	A	154	ARG	CD-NE-CZ	-9.38	111.27	124.40
1	A	86	HIS	CA-CB-CG	9.35	123.15	113.80
1	A	103	PHE	CA-CB-CG	9.24	123.04	113.80
1	A	181	MET	CA-CB-CG	9.14	132.39	114.10
1	A	67	ARG	CD-NE-CZ	-9.11	111.64	124.40
1	A	124	PHE	CA-C-N	-9.01	108.37	122.87
1	A	124	PHE	C-N-CA	-9.01	108.37	122.87
1	A	194	MET	CA-C-N	8.71	136.27	122.33
1	A	194	MET	C-N-CA	8.71	136.27	122.33
1	A	214	ALA	CB-CA-C	-8.71	94.59	109.83
1	A	229	ARG	CD-NE-CZ	-8.65	112.28	124.40
1	A	256	ASN	CA-C-O	8.62	130.67	121.45
1	A	195	VAL	N-CA-CB	-8.61	96.47	111.63
1	A	28	ALA	CA-C-O	-8.56	111.30	120.80
1	A	144	GLN	O-C-N	8.53	133.73	122.56
1	A	191	THR	CA-C-O	-8.52	111.13	120.92
1	A	267	ALA	CA-C-O	-8.50	111.54	120.55
1	A	205	GLU	CB-CG-CD	8.48	127.02	112.60
1	A	48	PHE	CA-C-O	-8.48	111.25	120.24
1	A	49	ASP	CA-CB-CG	8.37	120.97	112.60
1	A	48	PHE	CA-CB-CG	8.32	122.12	113.80
1	A	160	PRO	CA-C-O	-8.28	111.56	121.67
1	A	282	ILE	O-C-N	8.27	128.76	121.57
1	A	241	ILE	O-C-N	-8.21	113.73	122.68
1	A	164	ASP	CB-CA-C	-8.20	94.11	110.42
1	A	123	LYS	CA-CB-CG	8.19	130.49	114.10
1	A	171	ARG	NE-CZ-NH2	8.19	126.57	119.20
1	A	165	ALA	N-CA-C	8.17	120.92	111.11
1	A	185	ARG	NE-CZ-NH1	-8.10	113.40	121.50
1	A	80	MET	CA-CB-CG	8.10	130.30	114.10
1	A	46	GLN	CA-C-N	8.07	132.78	122.37
1	A	46	GLN	C-N-CA	8.07	132.78	122.37
1	A	96	VAL	CA-C-N	7.99	135.12	121.14
1	A	96	VAL	C-N-CA	7.99	135.12	121.14
1	A	118	GLY	CA-C-N	-7.98	110.35	121.13
1	A	118	GLY	C-N-CA	-7.98	110.35	121.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	N-CA-C	7.97	126.11	108.88
1	A	88	TYR	CA-CB-CG	7.97	128.25	113.90
1	A	236	PHE	CA-C-O	-7.94	112.16	120.89
1	A	58	ARG	CA-C-O	-7.93	112.67	121.87
1	A	91	TYR	N-CA-C	7.92	121.14	109.50
1	A	228	ALA	N-CA-C	-7.91	101.04	111.24
1	A	52	GLU	CA-C-O	-7.86	110.93	119.97
1	A	155	PHE	CA-C-N	-7.80	109.20	121.37
1	A	155	PHE	C-N-CA	-7.80	109.20	121.37
1	A	270	LYS	O-C-N	7.80	131.87	122.27
1	A	213	GLY	CA-C-O	-7.73	111.01	119.82
1	A	172	GLN	N-CA-C	-7.71	101.99	111.40
1	A	74	ASN	OD1-CG-ND2	7.70	130.30	122.60
1	A	164	ASP	N-CA-C	7.69	127.19	110.80
1	A	101	ARG	CA-C-O	-7.67	112.76	120.82
1	A	15	GLU	CA-CB-CG	7.63	129.37	114.10
1	A	76	ARG	CD-NE-CZ	-7.62	113.73	124.40
1	A	154	ARG	NE-CZ-NH1	-7.56	113.94	121.50
1	A	8	GLU	CA-C-O	-7.55	111.74	120.20
1	A	31	CYS	CA-C-N	7.54	136.20	121.41
1	A	31	CYS	C-N-CA	7.54	136.20	121.41
1	A	101	ARG	NE-CZ-NH1	7.54	129.04	121.50
1	A	60	THR	CA-CB-CG2	7.50	123.25	110.50
1	A	109	ASP	N-CA-C	-7.49	104.38	113.97
1	A	197	GLY	O-C-N	7.47	129.24	121.77
1	A	222	VAL	O-C-N	-7.47	112.59	121.10
1	A	47	ILE	N-CA-C	7.44	119.29	108.58
1	A	276	SER	CA-C-O	-7.43	112.54	120.42
1	A	133	ARG	O-C-N	7.42	131.45	122.48
1	A	163	SER	N-CA-C	-7.39	102.00	111.02
1	A	25	PRO	CA-C-O	-7.37	112.90	122.19
1	A	144	GLN	CA-C-O	-7.36	113.44	122.64
1	A	79	VAL	N-CA-CB	7.33	124.14	111.39
1	A	217	VAL	CA-C-O	-7.29	113.55	121.28
1	A	239	SER	CA-C-O	-7.29	112.50	120.30
1	A	20	HIS	O-C-N	7.28	129.65	121.93
1	A	204	ALA	CA-C-O	-7.23	113.45	120.90
1	A	221	THR	CA-C-O	-7.21	110.20	120.51
1	A	94	TRP	N-CA-C	-7.21	104.37	113.02
1	A	79	VAL	CB-CA-C	-7.19	99.90	110.62
1	A	185	ARG	NE-CZ-NH2	7.13	125.62	119.20
1	A	55	ASN	OD1-CG-ND2	7.12	129.72	122.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	HIS	CA-CB-CG	7.10	120.90	113.80
1	A	135	HIS	CA-C-O	7.04	128.99	121.45
1	A	150	PRO	CA-C-O	-7.03	113.33	121.34
1	A	288	ALA	N-CA-CB	-7.03	99.84	110.73
1	A	69	VAL	CA-C-O	-7.01	112.95	120.59
1	A	178	TRP	N-CA-C	-6.99	104.01	112.54
1	A	192	TYR	CA-C-O	-6.99	112.63	120.32
1	A	186	GLU	CA-C-N	6.99	133.52	122.34
1	A	186	GLU	C-N-CA	6.99	133.52	122.34
1	A	34	GLY	O-C-N	6.96	131.74	122.70
1	A	86	HIS	CA-C-N	6.94	129.58	120.28
1	A	86	HIS	C-N-CA	6.94	129.58	120.28
1	A	121	ASN	N-CA-C	-6.92	101.07	109.72
1	A	115	ASN	CA-C-O	-6.91	113.88	121.28
1	A	21	THR	N-CA-C	6.89	119.72	107.80
1	A	28	ALA	CA-C-N	-6.89	111.10	122.67
1	A	28	ALA	C-N-CA	-6.89	111.10	122.67
1	A	40	ASP	CA-C-N	6.84	132.14	120.72
1	A	40	ASP	C-N-CA	6.84	132.14	120.72
1	A	7	TYR	CA-C-O	-6.83	110.73	120.51
1	A	42	LEU	CA-C-O	-6.83	114.83	122.01
1	A	233	LEU	CB-CA-C	6.83	121.03	109.50
1	A	26	GLN	N-CA-C	-6.81	104.17	113.30
1	A	138	LEU	O-C-N	-6.78	113.53	121.32
1	A	194	MET	O-C-N	-6.75	115.33	123.10
1	A	54	PRO	O-C-N	-6.73	113.56	122.64
1	A	202	THR	CA-CB-CG2	6.70	121.89	110.50
1	A	132	ILE	N-CA-C	-6.70	99.99	109.63
1	A	74	ASN	CA-C-O	-6.69	113.85	122.14
1	A	69	VAL	CA-CB-CG1	6.67	121.75	110.40
1	A	49	ASP	CA-C-O	-6.67	114.29	121.56
1	A	246	ILE	CA-C-O	-6.67	112.89	120.95
1	A	126	VAL	CA-C-O	-6.66	113.49	121.28
1	A	161	ALA	CA-C-O	-6.65	114.11	121.89
1	A	72	PHE	CA-C-O	-6.65	112.09	120.20
1	A	10	TYR	N-CA-C	-6.64	103.66	111.03
1	A	204	ALA	CA-C-N	6.64	130.78	120.82
1	A	204	ALA	C-N-CA	6.64	130.78	120.82
1	A	9	ASP	O-C-N	6.61	129.69	122.15
1	A	115	ASN	CA-CB-CG	6.61	119.21	112.60
1	A	55	ASN	CA-C-O	-6.60	111.07	120.51
1	A	178	TRP	CA-CB-CG	6.59	126.12	113.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	HIS	O-C-N	6.58	129.09	122.12
1	A	171	ARG	NH1-CZ-NH2	-6.57	110.75	119.30
1	A	277	ILE	CA-CB-CG2	6.55	121.64	110.50
1	A	256	ASN	CA-C-N	6.53	130.78	121.71
1	A	256	ASN	C-N-CA	6.53	130.78	121.71
1	A	144	GLN	CB-CG-CD	-6.52	101.52	112.60
1	A	103	PHE	N-CA-C	-6.51	103.45	111.33
1	A	155	PHE	N-CA-C	-6.50	102.79	111.96
1	A	114	THR	O-C-N	6.50	130.38	123.03
1	A	92	PRO	CB-CA-C	6.50	119.50	111.12
1	A	145	ASN	CB-CA-C	6.50	118.94	108.87
1	A	51	SER	CA-C-N	6.47	130.15	120.31
1	A	51	SER	C-N-CA	6.47	130.15	120.31
1	A	141	PHE	N-CA-C	-6.47	104.27	111.71
1	A	193	VAL	CA-C-O	-6.47	113.65	120.57
1	A	215	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	44	GLN	N-CA-C	-6.39	105.43	113.23
1	A	108	VAL	CB-CA-C	6.39	120.98	111.26
1	A	137	ASN	O-C-N	-6.39	114.12	122.43
1	A	148	ARG	CB-CG-CD	6.38	125.98	111.30
1	A	175	LEU	CA-C-O	-6.38	114.06	121.07
1	A	52	GLU	N-CA-C	6.36	119.20	111.82
1	A	185	ARG	CD-NE-CZ	-6.36	115.50	124.40
1	A	119	GLY	N-CA-C	-6.35	102.92	113.02
1	A	288	ALA	CA-C-O	6.34	127.08	119.59
1	A	236	PHE	CB-CA-C	6.30	121.70	110.16
1	A	253	GLU	CA-CB-CG	6.30	126.71	114.10
1	A	29	ILE	O-C-N	6.30	129.65	123.03
1	A	160	PRO	CB-CA-C	6.29	119.22	110.98
1	A	106	LEU	CB-CA-C	6.28	120.83	110.90
1	A	20	HIS	CA-CB-CG	-6.28	107.52	113.80
1	A	79	VAL	N-CA-C	-6.27	99.45	108.48
1	A	222	VAL	CB-CA-C	6.27	122.77	111.36
1	A	214	ALA	CA-C-O	-6.26	114.34	121.72
1	A	74	ASN	N-CA-CB	-6.25	101.77	111.65
1	A	273	GLN	CA-CB-CG	6.24	126.57	114.10
1	A	8	GLU	N-CA-CB	6.23	119.99	110.14
1	A	175	LEU	CB-CA-C	6.21	120.80	110.92
1	A	257	HIS	O-C-N	6.21	129.09	122.38
1	A	152	ASP	CA-CB-CG	-6.20	106.41	112.60
1	A	85	PHE	CA-C-N	-6.19	111.95	123.03
1	A	85	PHE	C-N-CA	-6.19	111.95	123.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	PRO	CA-C-O	-6.18	109.35	120.60
1	A	241	ILE	CB-CG1-CD1	6.18	126.79	113.80
1	A	84	ARG	CD-NE-CZ	-6.17	115.76	124.40
1	A	52	GLU	CG-CD-OE1	-6.16	104.24	118.40
1	A	157	ASP	N-CA-CB	-6.14	100.11	110.49
1	A	199	SER	CA-C-O	-6.14	115.09	122.03
1	A	249	TYR	CB-CA-C	6.09	120.94	110.77
1	A	242	THR	CA-CB-OG1	-6.08	100.48	109.60
1	A	151	ASN	OD1-CG-ND2	-6.07	116.53	122.60
1	A	87	MET	CA-C-O	6.06	126.97	120.55
1	A	11	LYS	CA-CB-CG	6.04	126.18	114.10
1	A	287	LYS	CA-C-N	6.04	132.01	122.60
1	A	287	LYS	C-N-CA	6.04	132.01	122.60
1	A	47	ILE	CB-CA-C	-6.03	103.44	110.91
1	A	154	ARG	CG-CD-NE	6.03	125.26	112.00
1	A	67	ARG	O-C-N	6.02	129.58	123.26
1	A	245	VAL	CB-CA-C	6.00	121.13	111.29
1	A	147	LEU	N-CA-CB	-5.99	101.23	110.46
1	A	85	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	145	ASN	CA-C-N	5.96	125.51	119.19
1	A	145	ASN	C-N-CA	5.96	125.51	119.19
1	A	76	ARG	CA-C-N	5.95	130.86	121.99
1	A	76	ARG	C-N-CA	5.95	130.86	121.99
1	A	97	THR	N-CA-CB	-5.95	100.70	110.40
1	A	80	MET	CB-CA-C	5.94	121.11	109.35
1	A	233	LEU	N-CA-C	-5.94	100.61	110.17
1	A	113	VAL	CA-CB-CG1	5.93	120.47	110.40
1	A	268	ALA	N-CA-CB	5.90	119.31	110.22
1	A	29	ILE	N-CA-C	-5.88	99.80	108.85
1	A	202	THR	CA-C-O	-5.86	112.13	120.51
1	A	206	CYS	N-CA-C	-5.85	104.09	111.11
1	A	133	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	A	229	ARG	O-C-N	-5.84	115.39	122.22
1	A	253	GLU	CA-C-N	5.84	132.69	121.54
1	A	253	GLU	C-N-CA	5.84	132.69	121.54
1	A	241	ILE	CA-C-O	5.82	127.92	120.76
1	A	195	VAL	CA-C-O	-5.82	114.41	120.64
1	A	10	TYR	N-CA-CB	5.80	118.39	109.98
1	A	256	ASN	N-CA-C	5.79	117.58	108.96
1	A	23	HIS	CA-C-N	5.79	129.87	122.64
1	A	23	HIS	C-N-CA	5.79	129.87	122.64
1	A	168	ARG	NE-CZ-NH1	5.77	127.27	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	LYS	N-CA-C	-5.76	105.00	111.28
1	A	10	TYR	O-C-N	5.75	128.24	122.03
1	A	132	ILE	CA-C-O	-5.74	115.05	121.36
1	A	222	VAL	CA-C-N	5.74	127.02	119.84
1	A	222	VAL	C-N-CA	5.74	127.02	119.84
1	A	8	GLU	CB-CA-C	-5.73	99.33	110.46
1	A	11	LYS	CG-CD-CE	5.70	124.41	111.30
1	A	27	VAL	CA-C-O	-5.69	114.23	120.43
1	A	279	MET	CA-C-N	5.69	128.96	120.31
1	A	279	MET	C-N-CA	5.69	128.96	120.31
1	A	57	PRO	CA-C-N	5.69	131.32	120.97
1	A	57	PRO	C-N-CA	5.69	131.32	120.97
1	A	12	ASN	CA-C-O	-5.68	112.39	120.51
1	A	235	VAL	O-C-N	5.68	129.31	123.18
1	A	270	LYS	CA-C-O	-5.66	113.46	119.97
1	A	153	GLU	CA-CB-CG	5.63	125.36	114.10
1	A	165	ALA	CA-C-N	5.63	131.10	122.77
1	A	165	ALA	C-N-CA	5.63	131.10	122.77
1	A	263	ALA	CA-C-N	-5.62	110.39	121.41
1	A	263	ALA	C-N-CA	-5.62	110.39	121.41
1	A	195	VAL	CA-CB-CG1	5.62	119.95	110.40
1	A	183	GLU	N-CA-C	5.62	117.95	110.53
1	A	207	ARG	CB-CG-CD	5.62	124.22	111.30
1	A	273	GLN	OE1-CD-NE2	-5.60	117.00	122.60
1	A	120	LEU	O-C-N	5.60	127.96	122.19
1	A	117	ALA	CA-C-N	5.58	132.34	121.41
1	A	117	ALA	C-N-CA	5.58	132.34	121.41
1	A	212	LEU	CA-C-O	5.58	126.13	119.10
1	A	175	LEU	O-C-N	5.58	128.04	122.08
1	A	236	PHE	CA-CB-CG	5.57	119.37	113.80
1	A	278	LEU	CA-C-O	5.53	125.23	119.14
1	A	20	HIS	N-CA-C	-5.53	106.24	114.64
1	A	112	VAL	CA-C-O	-5.51	114.67	120.57
1	A	130	MET	CA-CB-CG	-5.49	103.12	114.10
1	A	194	MET	CA-C-O	5.48	127.75	121.28
1	A	239	SER	CA-CB-OG	-5.48	100.14	111.10
1	A	257	HIS	CB-CA-C	-5.48	102.19	112.00
1	A	284	LEU	CB-CA-C	5.48	116.82	109.42
1	A	129	ILE	CB-CA-C	5.43	118.26	110.33
1	A	48	PHE	O-C-N	5.43	129.62	123.27
1	A	125	GLU	CA-C-O	-5.43	115.03	121.16
1	A	160	PRO	O-C-N	5.43	129.73	123.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	CB-CA-C	-5.43	99.62	110.42
1	A	205	GLU	OE1-CD-OE2	-5.42	109.89	122.90
1	A	151	ASN	CA-CB-CG	5.41	118.01	112.60
1	A	131	LEU	N-CA-C	-5.40	99.72	108.41
1	A	144	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	261	LEU	CA-C-O	-5.36	112.84	120.51
1	A	205	GLU	CA-C-O	-5.36	114.92	120.92
1	A	110	THR	CA-C-O	-5.35	115.06	121.11
1	A	148	ARG	NH1-CZ-NH2	-5.35	112.34	119.30
1	A	226	ILE	N-CA-C	5.35	115.98	110.36
1	A	78	CYS	CA-C-N	5.34	130.43	123.06
1	A	78	CYS	C-N-CA	5.34	130.43	123.06
1	A	91	TYR	CB-CA-C	-5.32	100.90	109.67
1	A	45	ALA	O-C-N	5.31	129.45	122.97
1	A	52	GLU	CB-CA-C	-5.30	100.50	110.67
1	A	79	VAL	CA-C-N	-5.29	114.17	122.73
1	A	79	VAL	C-N-CA	-5.29	114.17	122.73
1	A	151	ASN	O-C-N	5.28	128.93	122.96
1	A	40	ASP	CB-CA-C	5.28	120.80	110.67
1	A	286	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	238	PHE	CA-CB-CG	-5.27	108.53	113.80
1	A	59	SER	N-CA-C	5.27	117.67	110.55
1	A	17	LEU	CA-C-O	-5.27	114.94	120.63
1	A	84	ARG	CA-C-O	-5.26	113.84	120.84
1	A	41	LYS	N-CA-C	5.26	118.96	112.54
1	A	274	PHE	CA-C-O	5.25	126.33	120.82
1	A	118	GLY	N-CA-C	-5.25	100.74	113.18
1	A	268	ALA	CA-C-O	-5.25	114.17	120.10
1	A	155	PHE	O-C-N	5.24	128.37	122.19
1	A	246	ILE	O-C-N	5.24	128.69	122.66
1	A	271	LEU	CB-CA-C	5.22	120.26	110.70
1	A	192	TYR	CB-CA-C	-5.21	101.64	110.19
1	A	220	SER	CA-C-N	5.21	131.49	121.54
1	A	220	SER	C-N-CA	5.21	131.49	121.54
1	A	5	TYR	CA-C-O	-5.20	114.60	120.32
1	A	61	VAL	CA-C-O	-5.20	112.98	119.95
1	A	105	LEU	O-C-N	-5.18	115.70	122.59
1	A	200	PHE	CA-C-O	5.18	127.98	121.66
1	A	89	GLU	CA-C-O	-5.17	112.49	119.11
1	A	33	SER	CA-C-N	5.17	131.54	121.41
1	A	33	SER	C-N-CA	5.17	131.54	121.41
1	A	19	SER	N-CA-C	-5.15	105.71	112.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	105	LEU	N-CA-CB	-5.15	101.79	110.49
1	A	107	GLY	CA-C-N	5.14	128.06	120.91
1	A	107	GLY	C-N-CA	5.14	128.06	120.91
1	A	64	HIS	CA-C-N	-5.14	115.53	123.14
1	A	64	HIS	C-N-CA	-5.14	115.53	123.14
1	A	133	ARG	N-CA-C	-5.14	107.39	113.97
1	A	208	VAL	CA-CB-CG2	5.12	119.11	110.40
1	A	80	MET	N-CA-CB	-5.12	101.73	111.00
1	A	206	CYS	CA-C-O	-5.11	115.43	120.90
1	A	236	PHE	N-CA-C	-5.11	100.69	108.76
1	A	96	VAL	O-C-N	-5.10	116.89	121.89
1	A	220	SER	CA-C-O	5.10	126.81	121.25
1	A	31	CYS	N-CA-CB	-5.08	102.14	110.43
1	A	232	GLY	CA-C-N	-5.08	114.00	122.64
1	A	232	GLY	C-N-CA	-5.08	114.00	122.64
1	A	46	GLN	CA-C-O	-5.07	113.63	120.47
1	A	170	MET	N-CA-C	-5.06	106.37	112.54
1	A	33	SER	O-C-N	5.04	129.30	122.59
1	A	167	ASP	CA-CB-CG	-5.02	107.58	112.60
1	A	61	VAL	N-CA-CB	-5.01	104.20	111.21

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	ARG	Sidechain
1	A	229	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	2258	0	2235	186	1
2	A	10	0	0	2	0
All	All	2268	0	2235	186	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 41.

All (186) 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:GLU:HG2	1:A:264:GLY:HA3	1.18	1.15
1:A:210:GLN:NE2	1:A:247:MET:HE3	1.64	1.12
1:A:210:GLN:CD	1:A:247:MET:CE	2.25	1.09
1:A:210:GLN:CD	1:A:247:MET:HE1	1.79	1.08
1:A:258:GLU:CG	1:A:264:GLY:HA3	1.93	0.98
1:A:42:LEU:HD11	1:A:80:MET:HE3	1.46	0.97
1:A:210:GLN:NE2	1:A:247:MET:CE	2.26	0.97
1:A:92:PRO:HD2	1:A:95:LYS:HD2	1.53	0.91
1:A:117:ALA:HB1	1:A:216:ALA:HB1	1.55	0.89
1:A:34:GLY:HA3	1:A:258:GLU:CD	1.98	0.88
1:A:136:ILE:HB	1:A:193:VAL:HG23	1.57	0.85
1:A:210:GLN:HE22	1:A:247:MET:HE3	1.37	0.84
1:A:21:THR:HG23	1:A:48:PHE:HZ	1.44	0.81
1:A:60:THR:O	1:A:62:PRO:HD2	1.82	0.79
1:A:42:LEU:HD22	1:A:71:GLY:HA3	1.63	0.79
1:A:165:ALA:HA	1:A:229:ARG:HD2	1.64	0.79
1:A:60:THR:HB	1:A:61:VAL:HG23	1.65	0.79
1:A:39:THR:HG22	1:A:80:MET:HG2	1.66	0.78
1:A:35:LEU:HD21	1:A:271:LEU:HD22	1.66	0.77
1:A:210:GLN:CD	1:A:247:MET:HE3	1.99	0.77
1:A:203:VAL:O	1:A:207:ARG:HG3	1.84	0.76
1:A:47:ILE:HD12	1:A:67:ARG:NH2	2.04	0.73
1:A:58:ARG:HH11	1:A:58:ARG:HG2	1.54	0.73
1:A:32:GLY:O	1:A:33:SER:C	2.32	0.73
1:A:139:PRO:O	1:A:144:GLN:HB2	1.89	0.71
1:A:86:HIS:N	1:A:89:GLU:OE2	2.22	0.71
1:A:210:GLN:OE1	1:A:247:MET:CE	2.37	0.71
1:A:21:THR:HG23	1:A:48:PHE:CZ	2.24	0.71
1:A:179:LYS:HG3	1:A:180:GLN:N	2.04	0.70
1:A:221:THR:O	1:A:225:VAL:HG23	1.93	0.69
1:A:57:PRO:HG2	1:A:85:PHE:CE2	2.28	0.69
1:A:97:THR:HG23	1:A:227:VAL:HG21	1.74	0.69
1:A:132:ILE:HG23	1:A:192:TYR:HB2	1.74	0.69
1:A:149:GLY:O	1:A:158:ARG:NH2	2.25	0.69
1:A:236:PHE:HE1	1:A:238:PHE:CZ	2.10	0.69
1:A:97:THR:HG21	1:A:227:VAL:HG11	1.76	0.68
1:A:35:LEU:HD21	1:A:271:LEU:CD2	2.24	0.68
1:A:206:CYS:SG	1:A:245:VAL:HG12	2.34	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:THR:CG2	1:A:227:VAL:HG21	2.24	0.67
1:A:225:VAL:HG13	1:A:235:VAL:HG11	1.77	0.67
1:A:34:GLY:HA2	2:A:291:SO4:O4	1.95	0.66
1:A:271:LEU:C	1:A:271:LEU:HD23	2.21	0.66
1:A:60:THR:C	1:A:62:PRO:HD2	2.22	0.65
1:A:81:MET:HG3	1:A:103:PHE:HZ	1.61	0.65
1:A:206:CYS:SG	1:A:245:VAL:CG1	2.85	0.64
1:A:129:ILE:HD13	1:A:271:LEU:HB2	1.79	0.64
1:A:285:PRO:O	1:A:287:LYS:N	2.30	0.64
1:A:179:LYS:CG	1:A:180:GLN:N	2.61	0.64
1:A:179:LYS:O	1:A:182:GLY:N	2.30	0.63
1:A:28:ALA:HB3	1:A:111:LEU:HD12	1.80	0.63
1:A:210:GLN:CB	1:A:247:MET:HE1	2.28	0.62
1:A:66:GLY:HA2	1:A:82:GLN:O	2.00	0.60
1:A:268:ALA:O	1:A:272:GLU:HG3	2.02	0.59
1:A:34:GLY:HA3	1:A:258:GLU:OE2	2.01	0.59
1:A:99:PRO:O	1:A:100:VAL:C	2.44	0.59
1:A:135:HIS:HA	1:A:192:TYR:O	2.03	0.59
1:A:18:LEU:HD13	1:A:106:LEU:HD12	1.85	0.59
1:A:93:LEU:HA	1:A:96:VAL:HG13	1.85	0.58
1:A:127:GLY:HA2	1:A:267:ALA:HB2	1.85	0.58
1:A:31:CYS:HB2	1:A:81:MET:O	2.03	0.58
1:A:57:PRO:HG2	1:A:85:PHE:HE2	1.68	0.58
1:A:211:LYS:C	1:A:213:GLY:H	2.11	0.57
1:A:246:ILE:HD12	1:A:250:GLU:CD	2.30	0.57
1:A:162:MET:O	1:A:163:SER:C	2.44	0.57
1:A:34:GLY:HA3	1:A:258:GLU:OE1	2.04	0.57
1:A:210:GLN:HB2	1:A:247:MET:HE1	1.86	0.57
1:A:102:VAL:O	1:A:103:PHE:C	2.48	0.57
1:A:117:ALA:CB	1:A:216:ALA:HB1	2.33	0.57
1:A:51:SER:HA	1:A:58:ARG:HD3	1.86	0.57
1:A:42:LEU:CD1	1:A:80:MET:HE3	2.30	0.56
1:A:56:PHE:O	1:A:57:PRO:C	2.49	0.56
1:A:176:SER:O	1:A:179:LYS:N	2.34	0.56
1:A:28:ALA:HB1	1:A:103:PHE:CE2	2.41	0.56
1:A:284:LEU:C	1:A:284:LEU:HD23	2.31	0.55
1:A:114:THR:O	1:A:115:ASN:HB3	2.06	0.55
1:A:26:GLN:O	1:A:26:GLN:HG2	2.05	0.55
1:A:97:THR:HG23	1:A:227:VAL:CG2	2.37	0.55
1:A:42:LEU:HD22	1:A:71:GLY:CA	2.36	0.54
1:A:43:THR:O	1:A:44:GLN:HB2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:HIS:CE1	1:A:222:VAL:HG13	2.43	0.54
1:A:183:GLU:OE2	1:A:270:LYS:HD2	2.08	0.54
1:A:97:THR:CG2	1:A:227:VAL:HG11	2.37	0.53
1:A:285:PRO:O	1:A:287:LYS:HG3	2.08	0.53
1:A:252:LEU:HD12	1:A:252:LEU:O	2.09	0.53
1:A:204:ALA:O	1:A:207:ARG:N	2.41	0.53
1:A:115:ASN:HB2	2:A:290:SO4:O3	2.09	0.53
1:A:93:LEU:HD22	1:A:223:PRO:HG3	1.91	0.52
1:A:274:PHE:O	1:A:278:LEU:HD12	2.08	0.52
1:A:30:ILE:O	1:A:114:THR:OG1	2.23	0.52
1:A:258:GLU:HA	1:A:264:GLY:H	1.75	0.52
1:A:138:LEU:N	1:A:139:PRO:CD	2.73	0.51
1:A:179:LYS:CG	1:A:180:GLN:H	2.22	0.51
1:A:124:PHE:O	1:A:244:LYS:HD2	2.10	0.51
1:A:211:LYS:C	1:A:213:GLY:N	2.69	0.51
1:A:32:GLY:O	1:A:35:LEU:HB2	2.11	0.51
1:A:3:ASN:C	1:A:5:TYR:H	2.18	0.50
1:A:252:LEU:HD12	1:A:252:LEU:C	2.37	0.50
1:A:21:THR:HG22	1:A:46:GLN:CD	2.36	0.50
1:A:130:MET:HE3	1:A:190:GLY:O	2.12	0.50
1:A:207:ARG:O	1:A:211:LYS:HG2	2.12	0.50
1:A:284:LEU:O	1:A:287:LYS:HG3	2.11	0.50
1:A:29:ILE:HG12	1:A:112:VAL:HG13	1.94	0.49
1:A:35:LEU:C	1:A:37:GLY:N	2.68	0.49
1:A:101:ARG:O	1:A:104:HIS:HB3	2.12	0.49
1:A:284:LEU:O	1:A:285:PRO:C	2.56	0.49
1:A:138:LEU:O	1:A:139:PRO:C	2.53	0.49
1:A:131:LEU:HD11	1:A:171:ARG:HG2	1.94	0.49
1:A:177:THR:HA	1:A:180:GLN:HB2	1.95	0.48
1:A:50:TYR:O	1:A:52:GLU:N	2.47	0.48
1:A:103:PHE:O	1:A:104:HIS:C	2.55	0.48
1:A:222:VAL:O	1:A:223:PRO:C	2.55	0.48
1:A:187:LEU:HD13	1:A:274:PHE:CE2	2.48	0.48
1:A:11:LYS:O	1:A:12:ASN:C	2.55	0.48
1:A:264:GLY:O	1:A:268:ALA:CB	2.62	0.48
1:A:25:PRO:HG3	1:A:79:VAL:HG22	1.95	0.48
1:A:123:LYS:O	1:A:124:PHE:CD1	2.67	0.48
1:A:22:LYS:HE2	1:A:23:HIS:CD2	2.49	0.47
1:A:169:THR:O	1:A:173:ARG:HB2	2.14	0.47
1:A:265:LYS:O	1:A:266:GLN:C	2.57	0.47
1:A:170:MET:CE	1:A:282:ILE:HG13	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:HB2	1:A:206:CYS:SG	2.54	0.47
1:A:138:LEU:HB2	1:A:139:PRO:HD3	1.96	0.47
1:A:262:ALA:O	1:A:266:GLN:N	2.48	0.47
1:A:236:PHE:HE1	1:A:238:PHE:HZ	1.59	0.46
1:A:10:TYR:O	1:A:11:LYS:C	2.58	0.46
1:A:14:ALA:O	1:A:17:LEU:N	2.48	0.46
1:A:132:ILE:CG2	1:A:192:TYR:HB2	2.42	0.46
1:A:222:VAL:O	1:A:226:ILE:HG13	2.15	0.46
1:A:228:ALA:O	1:A:231:CYS:HB2	2.16	0.46
1:A:39:THR:HB	1:A:69:VAL:HG11	1.98	0.46
1:A:152:ASP:OD1	1:A:152:ASP:C	2.58	0.46
1:A:236:PHE:CE1	1:A:238:PHE:CZ	2.97	0.46
1:A:81:MET:HE2	1:A:81:MET:HB3	1.77	0.45
1:A:43:THR:O	1:A:44:GLN:CB	2.63	0.45
1:A:42:LEU:CD2	1:A:71:GLY:HA3	2.40	0.45
1:A:57:PRO:HB3	1:A:95:LYS:HG2	1.99	0.45
1:A:112:VAL:HA	1:A:236:PHE:O	2.16	0.45
1:A:98:PHE:N	1:A:99:PRO:CD	2.80	0.45
1:A:147:LEU:HD22	1:A:226:ILE:CG2	2.46	0.45
1:A:131:LEU:O	1:A:132:ILE:C	2.57	0.45
1:A:277:ILE:CG2	1:A:277:ILE:O	2.65	0.45
1:A:151:ASN:HD21	1:A:157:ASP:C	2.25	0.44
1:A:151:ASN:ND2	1:A:157:ASP:O	2.51	0.44
1:A:224:GLU:O	1:A:228:ALA:HB2	2.16	0.44
1:A:193:VAL:O	1:A:193:VAL:HG13	2.18	0.44
1:A:32:GLY:O	1:A:33:SER:O	2.36	0.44
1:A:206:CYS:SG	1:A:245:VAL:HG11	2.58	0.44
1:A:94:TRP:CZ3	1:A:95:LYS:HE2	2.53	0.44
1:A:152:ASP:O	1:A:155:PHE:N	2.36	0.44
1:A:116:ALA:HB1	1:A:242:THR:CG2	2.48	0.44
1:A:246:ILE:HG22	1:A:248:ASP:H	1.82	0.43
1:A:35:LEU:C	1:A:37:GLY:H	2.26	0.43
1:A:117:ALA:HB3	1:A:241:ILE:HD12	2.00	0.43
1:A:284:LEU:HD23	1:A:285:PRO:N	2.34	0.43
1:A:25:PRO:CG	1:A:79:VAL:HG22	2.48	0.43
1:A:149:GLY:O	1:A:158:ARG:NH1	2.47	0.43
1:A:210:GLN:CG	1:A:247:MET:HE1	2.47	0.43
1:A:180:GLN:HE21	1:A:180:GLN:HB3	1.42	0.43
1:A:14:ALA:O	1:A:15:GLU:C	2.61	0.43
1:A:133:ARG:O	1:A:133:ARG:CG	2.66	0.43
1:A:133:ARG:O	1:A:133:ARG:HG2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:MET:HE3	1:A:190:GLY:C	2.44	0.42
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.91	0.42
1:A:21:THR:C	1:A:23:HIS:H	2.27	0.42
1:A:129:ILE:HG12	1:A:240:LEU:HD12	2.02	0.42
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.27	0.42
1:A:46:GLN:N	1:A:70:PHE:O	2.49	0.42
1:A:109:ASP:OD1	1:A:234:ARG:NH2	2.52	0.42
1:A:205:GLU:O	1:A:206:CYS:C	2.62	0.42
1:A:80:MET:HB2	1:A:80:MET:HE2	1.67	0.42
1:A:10:TYR:CD2	1:A:155:PHE:HZ	2.38	0.41
1:A:93:LEU:CD2	1:A:223:PRO:HG3	2.50	0.41
1:A:125:GLU:O	1:A:126:VAL:C	2.63	0.41
1:A:28:ALA:CB	1:A:103:PHE:CD2	3.03	0.41
1:A:144:GLN:OE1	1:A:144:GLN:HA	2.21	0.41
1:A:115:ASN:ND2	1:A:239:SER:OG	2.52	0.41
1:A:70:PHE:CD1	1:A:70:PHE:N	2.89	0.41
1:A:258:GLU:HA	1:A:264:GLY:N	2.36	0.41
1:A:10:TYR:O	1:A:13:THR:N	2.54	0.40
1:A:211:LYS:O	1:A:213:GLY:N	2.54	0.40
1:A:3:ASN:C	1:A:5:TYR:N	2.73	0.40
1:A:67:ARG:HG3	1:A:67:ARG:NH1	2.34	0.40
1:A:161:ALA:C	1:A:162:MET:HG2	2.46	0.40
1:A:152:ASP:HB3	1:A:155:PHE:HD2	1.87	0.40
1:A:135:HIS:ND1	1:A:222:VAL:HG13	2.36	0.40
1:A:282:ILE:C	1:A:283:PRO:O	2.62	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:75:GLY:O	1:A:180:GLN:OE1[12_555]	2.06	0.14

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	287/289 (99%)	223 (78%)	44 (15%)	20 (7%)	1	1

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	54	PRO
1	A	196	ALA
1	A	197	GLY
1	A	254	LYS
1	A	184	GLN
1	A	260	VAL
1	A	286	ASP
1	A	61	VAL
1	A	104	HIS
1	A	164	ASP
1	A	266	GLN
1	A	50	TYR
1	A	202	THR
1	A	105	LEU
1	A	167	ASP
1	A	255	ALA
1	A	223	PRO
1	A	4	GLY
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	240/240 (100%)	166 (69%)	74 (31%)	0	0

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	13	THR
1	A	15	GLU
1	A	18	LEU
1	A	22	LYS
1	A	25	PRO
1	A	35	LEU
1	A	38	LEU
1	A	42	LEU
1	A	47	ILE
1	A	51	SER
1	A	56	PHE
1	A	58	ARG
1	A	59	SER
1	A	67	ARG
1	A	69	VAL
1	A	70	PHE
1	A	78	CYS
1	A	79	VAL
1	A	86	HIS
1	A	96	VAL
1	A	99	PRO
1	A	102	VAL
1	A	106	LEU
1	A	112	VAL
1	A	115	ASN
1	A	124	PHE
1	A	126	VAL
1	A	130	MET
1	A	131	LEU
1	A	135	HIS
1	A	136	ILE
1	A	139	PRO
1	A	141	PHE
1	A	142	SER
1	A	147	LEU
1	A	158	ARG
1	A	163	SER
1	A	164	ASP
1	A	167	ASP
1	A	168	ARG
1	A	171	ARG
1	A	172	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	173	ARG
1	A	177	THR
1	A	180	GLN
1	A	187	LEU
1	A	195	VAL
1	A	201	GLU
1	A	208	VAL
1	A	209	LEU
1	A	211	LYS
1	A	212	LEU
1	A	226	ILE
1	A	227	VAL
1	A	229	ARG
1	A	239	SER
1	A	241	ILE
1	A	243	ASN
1	A	244	LYS
1	A	245	VAL
1	A	247	MET
1	A	254	LYS
1	A	257	HIS
1	A	258	GLU
1	A	259	GLU
1	A	265	LYS
1	A	270	LYS
1	A	271	LEU
1	A	276	SER
1	A	277	ILE
1	A	278	LEU
1	A	283	PRO
1	A	286	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	74	ASN
1	A	115	ASN
1	A	137	ASN
1	A	151	ASN
1	A	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	0.74	0	6,6,6	0.61	0
2	SO4	A	290	-	4,4,4	1.08	0	6,6,6	1.58	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	290	SO4	O3-S-O2	2.79	124.12	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	291	SO4	1	0
2	A	290	SO4	1	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 ⓘ

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	289/289 (100%)	1.31	57 (19%) 3 2	8, 25, 54, 59	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	VAL	10.8
1	A	258	GLU	10.6
1	A	252	LEU	8.3
1	A	3	ASN	8.2
1	A	261	LEU	7.9
1	A	259	GLU	6.9
1	A	64	HIS	6.8
1	A	61	VAL	6.6
1	A	287	LYS	6.1
1	A	65	ALA	6.0
1	A	262	ALA	5.6
1	A	263	ALA	5.6
1	A	1	MET	5.4
1	A	255	ALA	5.1
1	A	257	HIS	5.1
1	A	254	LYS	4.9
1	A	286	ASP	4.9
1	A	256	ASN	4.8
1	A	2	GLU	4.8
1	A	288	ALA	4.7
1	A	248	ASP	4.7
1	A	180	GLN	4.4
1	A	185	ARG	4.3
1	A	253	GLU	3.9
1	A	289	SER	3.8
1	A	8	GLU	3.6
1	A	250	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	269	GLN	3.4
1	A	267	ALA	3.4
1	A	75	GLY	3.2
1	A	62	PRO	3.2
1	A	266	GLN	3.0
1	A	156	GLY	3.0
1	A	285	PRO	2.9
1	A	63	GLY	2.9
1	A	273	GLN	2.7
1	A	179	LYS	2.7
1	A	23	HIS	2.7
1	A	264	GLY	2.7
1	A	181	MET	2.6
1	A	58	ARG	2.6
1	A	251	SER	2.5
1	A	265	LYS	2.5
1	A	284	LEU	2.5
1	A	240	LEU	2.5
1	A	249	TYR	2.4
1	A	239	SER	2.4
1	A	59	SER	2.3
1	A	66	GLY	2.3
1	A	51	SER	2.2
1	A	19	SER	2.2
1	A	244	LYS	2.2
1	A	60	THR	2.2
1	A	113	VAL	2.2
1	A	281	SER	2.2
1	A	278	LEU	2.0
1	A	133	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no 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($\text{\AA}^2$)	Q<0.9
2	SO4	A	291	5/5	0.93	0.18	50,51,51,51	0
2	SO4	A	290	5/5	0.98	0.06	16,16,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.