



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:09 PM UTC

PDB ID : 5Z9X / pdb_00005z9x
Title : Arabidopsis SMALL RNA DEGRADING NUCLEASE 1 in complex with an RNA substrate
Authors : Chen, J.; Liu, L.; You, C.; Gu, J.; Ruan, W.; Zhang, L.; Gan, J.; Cao, C.; Huang, Y.; Chen, X.; Ma, J.
Deposited on : 2018-02-05
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 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

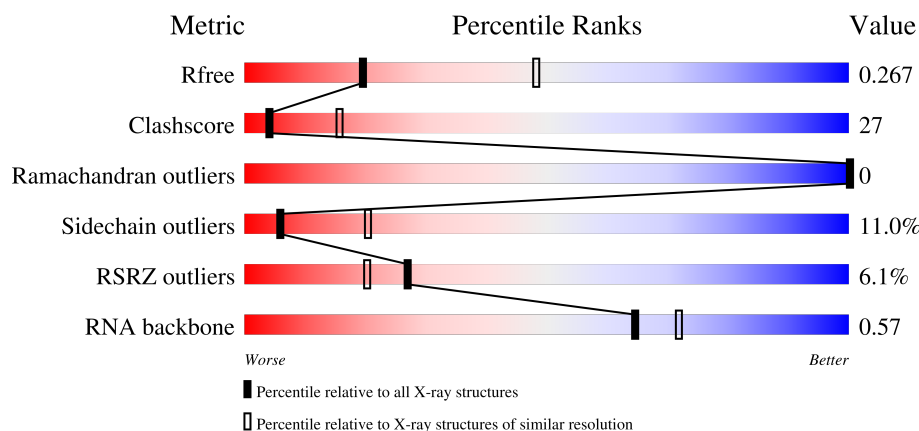
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	409	4% 30% 31% 8% • 30%
2	R	10	50% 40% 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2492 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.

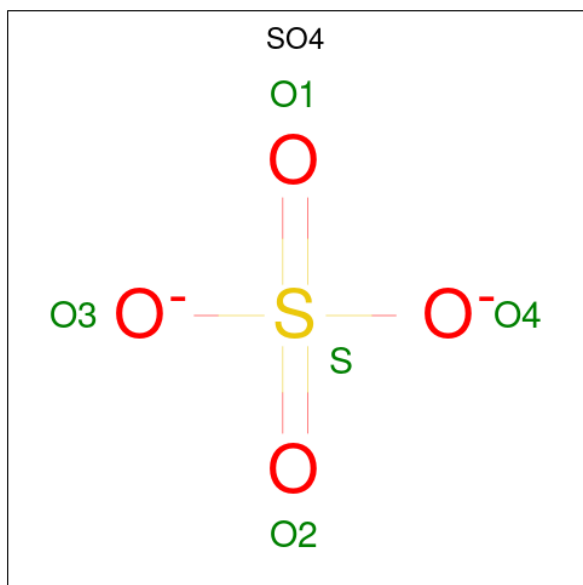
- Molecule 1 is a protein called Small RNA degrading nuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2263	1425	384	442	12	0	1	0

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*CP*CP*CP*AP*UP*UP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	R	9	190	85	33	63	9	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0

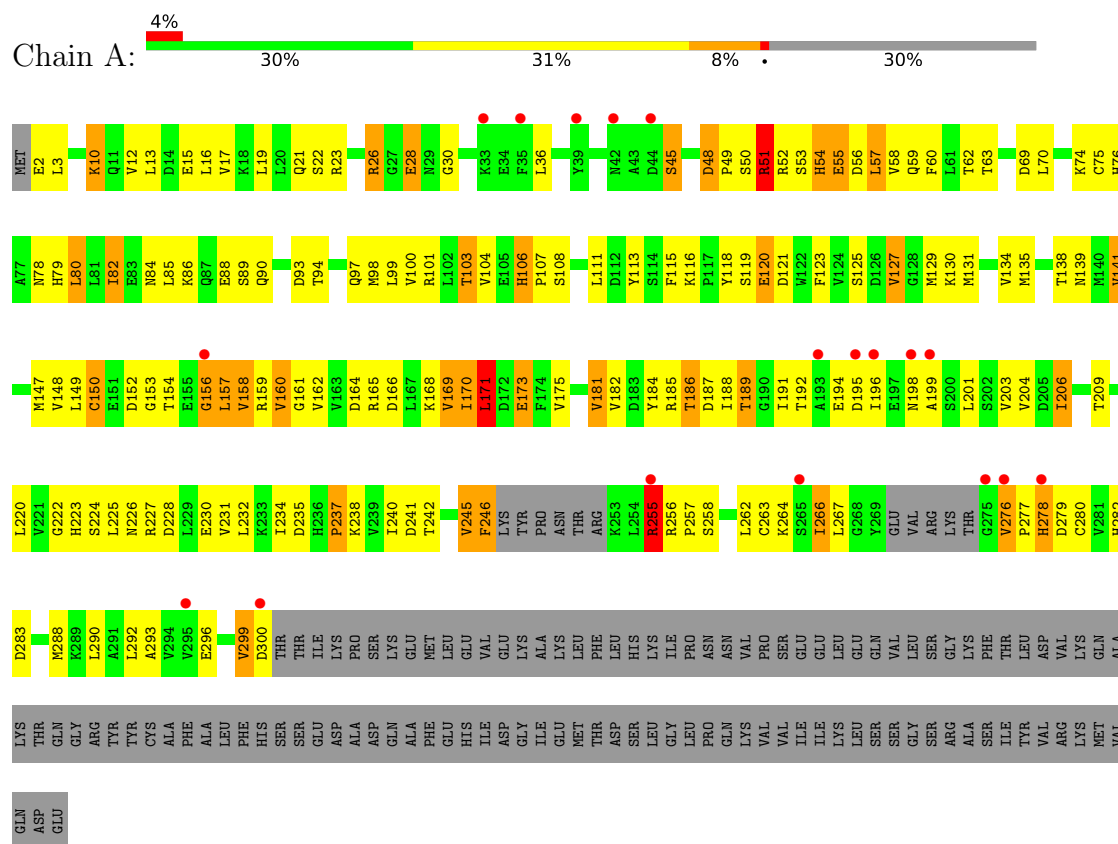
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	25	Total 25	O 25	0	0
5	R	2	Total 2	O 2	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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: Small RNA degrading nuclease 1



• Molecule 2: RNA (5'-R(P*GP*CP*CP*CP*AP*UP*UP*AP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.99Å 87.99Å 178.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.99 – 2.80 28.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.99-2.80) 99.3 (28.99-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.80Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.252 , 0.261 0.256 , 0.267	Depositor DCC
R_{free} test set	2001 reflections (9.85%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2492	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.07	8/2301 (0.3%)	1.42	44/3114 (1.4%)
2	R	0.32	0/211	0.58	0/326
All	All	1.03	8/2512 (0.3%)	1.37	44/3440 (1.3%)

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	3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ARG	CB-CG	8.30	1.77	1.52
1	A	255	ARG	CG-CD	7.20	1.74	1.52
1	A	170	ILE	C-O	-6.31	1.17	1.23
1	A	158	VAL	C-O	-6.24	1.17	1.23
1	A	45	SER	C-N	5.92	1.40	1.33
1	A	276	VAL	C-N	5.47	1.41	1.33
1	A	255	ARG	CZ-NH2	5.41	1.40	1.33
1	A	171	LEU	C-O	-5.11	1.17	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ILE	N-CA-C	14.78	124.52	111.81
1	A	52	ARG	N-CA-C	12.94	125.38	111.28
1	A	171	LEU	N-CA-C	-11.39	88.54	108.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ASP	N-CA-C	10.95	123.29	111.36
1	A	245	VAL	N-CA-C	9.48	119.44	110.53
1	A	55	GLU	CA-C-N	-9.19	107.97	120.28
1	A	55	GLU	C-N-CA	-9.19	107.97	120.28
1	A	57	LEU	N-CA-C	9.12	121.30	111.36
1	A	158	VAL	N-CA-C	8.96	119.16	111.90
1	A	266	ILE	N-CA-C	8.46	118.48	110.53
1	A	153	GLY	N-CA-C	-7.92	104.39	115.32
1	A	173	GLU	N-CA-C	7.45	120.39	109.07
1	A	48	ASP	CA-C-N	-7.10	112.32	121.91
1	A	48	ASP	C-N-CA	-7.10	112.32	121.91
1	A	51	ARG	CA-C-N	6.92	129.55	120.28
1	A	51	ARG	C-N-CA	6.92	129.55	120.28
1	A	106	HIS	CA-C-N	6.88	126.51	119.56
1	A	106	HIS	C-N-CA	6.88	126.51	119.56
1	A	45	SER	CA-C-N	-6.74	113.85	120.52
1	A	45	SER	C-N-CA	-6.74	113.85	120.52
1	A	161	GLY	CA-C-O	-6.73	115.69	120.94
1	A	276	VAL	CA-C-N	-6.58	113.00	119.78
1	A	276	VAL	C-N-CA	-6.58	113.00	119.78
1	A	111	LEU	N-CA-C	6.42	118.35	111.36
1	A	170	ILE	CB-CA-C	-6.20	104.42	111.55
1	A	186	THR	N-CA-C	-6.12	101.21	110.28
1	A	169	VAL	O-C-N	6.00	129.69	123.03
1	A	255	ARG	NE-CZ-NH1	-5.94	115.56	121.50
1	A	264	LYS	N-CA-C	-5.90	104.85	111.28
1	A	28	GLU	N-CA-C	-5.77	104.99	111.28
1	A	156	GLY	N-CA-C	5.70	119.45	110.96
1	A	170	ILE	CA-C-O	-5.63	114.12	120.32
1	A	138	THR	CA-C-N	-5.61	115.25	123.00
1	A	138	THR	C-N-CA	-5.61	115.25	123.00
1	A	227	ARG	N-CA-C	-5.60	105.26	111.36
1	A	157	LEU	CA-C-N	5.53	128.03	122.66
1	A	157	LEU	C-N-CA	5.53	128.03	122.66
1	A	55	GLU	N-CA-C	-5.48	105.30	111.28
1	A	120	GLU	N-CA-C	-5.43	105.95	112.58
1	A	278	HIS	N-CA-C	5.42	118.50	110.48
1	A	237	PRO	N-CA-C	5.41	121.05	113.53
1	A	120	GLU	CA-C-N	5.36	130.79	122.49
1	A	120	GLU	C-N-CA	5.36	130.79	122.49
1	A	21	GLN	N-CA-C	-5.11	105.60	111.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	GLU	Peptide
1	A	51	ARG	Peptide
1	A	90	GLN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2263	0	2244	130	0
2	R	190	0	98	5	0
3	A	5	0	0	1	0
3	R	5	0	0	0	0
4	A	2	0	0	0	0
5	A	25	0	0	9	0
5	R	2	0	0	1	0
All	All	2492	0	2342	132	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 27.

All (132) 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:255:ARG:CB	1:A:255:ARG:CG	1.77	1.56
1:A:129:MET:SD	5:A:625:HOH:O	2.37	0.83
1:A:164:ASP:HB3	1:A:170:ILE:HD11	1.59	0.82
1:A:99:LEU:HB3	1:A:240:ILE:HD12	1.61	0.81
1:A:263:CYS:O	1:A:267:LEU:N	2.15	0.79
1:A:23:ARG:NH2	5:A:602:HOH:O	2.17	0.78
1:A:48:ASP:O	1:A:50:SER:N	2.16	0.77
1:A:147:MET:HE3	2:R:10:G:H4'	1.68	0.75
1:A:48:ASP:C	1:A:50:SER:H	1.94	0.74
1:A:150:CYS:HB2	1:A:154:THR:O	1.88	0.73
1:A:23:ARG:NH1	3:A:501:SO4:O3	2.15	0.73
1:A:188:ILE:HG23	1:A:278:HIS:HB2	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:SER:O	1:A:54:HIS:C	2.31	0.72
1:A:53:SER:O	1:A:56:ASP:N	2.24	0.70
1:A:188:ILE:CG2	1:A:278:HIS:HB2	2.22	0.69
1:A:28:GLU:H	1:A:63:THR:HG22	1.57	0.69
1:A:97:GLN:HA	1:A:100:VAL:HG12	1.74	0.69
1:A:55:GLU:HA	1:A:58:VAL:HG22	1.75	0.68
1:A:3:LEU:HD13	1:A:70:LEU:HD22	1.76	0.67
1:A:258:SER:HB2	2:R:8:U:H5''	1.76	0.67
1:A:257:PRO:O	2:R:8:U:H4'	1.95	0.66
1:A:79:HIS:O	1:A:82:ILE:HG13	1.94	0.66
1:A:148:VAL:HG23	1:A:181:VAL:HG11	1.77	0.66
1:A:88:GLU:O	1:A:101:ARG:NH1	2.25	0.66
1:A:119:SER:OG	5:A:601:HOH:O	2.14	0.66
1:A:36:LEU:HD11	1:A:51:ARG:NH2	2.10	0.65
1:A:17:VAL:HG21	1:A:57:LEU:HD22	1.79	0.64
1:A:113:TYR:CE2	1:A:226:ASN:HB3	2.33	0.64
1:A:188:ILE:HG23	1:A:278:HIS:H	1.63	0.64
1:A:279:ASP:OD2	1:A:282:HIS:ND1	2.27	0.63
1:A:125:SER:OG	1:A:127:VAL:HG12	1.98	0.62
1:A:159:ARG:NH2	1:A:279:ASP:OD1	2.28	0.62
1:A:19:LEU:HD11	1:A:76:HIS:CG	2.35	0.61
1:A:188:ILE:O	1:A:188:ILE:HG22	2.00	0.61
1:A:28:GLU:N	1:A:63:THR:HG22	2.15	0.61
1:A:150:CYS:SG	1:A:181:VAL:HG13	2.42	0.60
1:A:164:ASP:OD1	1:A:168:LYS:N	2.34	0.60
1:A:171:LEU:HD22	1:A:209:THR:HG21	1.83	0.60
1:A:188:ILE:HG12	1:A:277:PRO:HA	1.84	0.59
1:A:115:PHE:N	5:A:603:HOH:O	2.36	0.58
1:A:160:VAL:HG21	1:A:206:ILE:HD11	1.84	0.58
1:A:59:GLN:O	1:A:62:THR:HG22	2.03	0.58
1:A:245:VAL:O	1:A:246:PHE:HB2	2.03	0.58
1:A:118:TYR:OH	1:A:235:ASP:OD2	2.22	0.58
1:A:232:LEU:HB3	1:A:234:ILE:HD12	1.84	0.58
1:A:60:PHE:O	1:A:63:THR:OG1	2.14	0.57
1:A:131:MET:HG2	1:A:134:VAL:HG23	1.87	0.55
1:A:54:HIS:O	1:A:57:LEU:N	2.40	0.54
1:A:93:ASP:OD1	1:A:97:GLN:HB3	2.08	0.54
1:A:12:VAL:HG12	1:A:16:LEU:HD11	1.89	0.54
1:A:103:THR:HG21	1:A:240:ILE:HA	1.88	0.54
1:A:184:TYR:CZ	1:A:192:THR:HB	2.43	0.53
1:A:98:MET:O	1:A:101:ARG:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:VAL:HG21	1:A:206:ILE:CD1	2.38	0.53
1:A:53:SER:O	1:A:55:GLU:N	2.41	0.53
1:A:53:SER:C	1:A:55:GLU:N	2.61	0.53
1:A:141:VAL:HG12	1:A:164:ASP:HA	1.90	0.52
2:R:5:C:H2'	2:R:6:A:C8	2.45	0.52
1:A:160:VAL:HG11	1:A:206:ILE:HD12	1.91	0.52
1:A:55:GLU:O	1:A:56:ASP:C	2.48	0.51
1:A:60:PHE:C	1:A:63:THR:HG1	2.14	0.51
1:A:74:LYS:HG2	1:A:129:MET:HE1	1.93	0.51
1:A:147:MET:HA	1:A:156:GLY:O	2.09	0.51
1:A:86:LYS:O	1:A:101:ARG:NH1	2.44	0.51
1:A:106:HIS:CD2	1:A:108:SER:H	2.29	0.51
1:A:106:HIS:HD2	1:A:108:SER:H	1.59	0.51
1:A:173:GLU:HG3	1:A:201:LEU:HD22	1.93	0.51
1:A:13:LEU:HA	1:A:16:LEU:HD12	1.91	0.50
1:A:80:LEU:HD23	5:A:605:HOH:O	2.11	0.50
1:A:150:CYS:HA	1:A:181:VAL:HG12	1.92	0.50
1:A:228:ASP:O	1:A:231:VAL:HG12	2.12	0.50
1:A:187:ASP:OD1	1:A:188:ILE:HG13	2.11	0.50
1:A:2:GLU:HG3	1:A:3:LEU:H	1.77	0.49
1:A:196:ILE:O	1:A:199:ALA:HB2	2.11	0.49
1:A:15:GLU:HG3	1:A:80:LEU:HD11	1.94	0.49
1:A:75:CYS:SG	1:A:116:LYS:HE3	2.52	0.49
1:A:26:ARG:HA	1:A:30:GLY:HA2	1.94	0.49
1:A:225:LEU:O	1:A:228:ASP:HB2	2.12	0.49
1:A:186:THR:HA	1:A:187:ASP:C	2.39	0.48
1:A:280:CYS:HA	1:A:283:ASP:HB2	1.95	0.48
1:A:135:MET:O	1:A:238:LYS:NZ	2.41	0.48
1:A:224:SER:N	1:A:241:ASP:OD1	2.40	0.48
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.49	0.48
1:A:165:ARG:NH2	5:A:607:HOH:O	2.46	0.48
1:A:223:HIS:ND1	1:A:242:THR:HB	2.29	0.48
1:A:162:VAL:HG23	1:A:171:LEU:HB3	1.95	0.47
1:A:94:THR:O	1:A:97:GLN:N	2.44	0.47
1:A:262:LEU:O	1:A:266:ILE:N	2.29	0.47
1:A:148:VAL:HA	1:A:185:ARG:HD2	1.97	0.47
1:A:186:THR:HG21	1:A:191:ILE:HD13	1.95	0.47
1:A:290:LEU:O	1:A:293:ALA:HB3	2.15	0.47
1:A:139:ASN:HA	5:A:607:HOH:O	2.15	0.47
1:A:148:VAL:CG2	1:A:181:VAL:HG11	2.45	0.47
1:A:194:GLU:O	1:A:198:ASN:ND2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TYR:OH	1:A:241:ASP:OD2	2.30	0.46
1:A:103:THR:O	1:A:103:THR:OG1	2.31	0.46
1:A:158:VAL:HA	1:A:175:VAL:O	2.15	0.46
1:A:187:ASP:CG	1:A:188:ILE:HG13	2.40	0.46
1:A:226:ASN:O	1:A:230:GLU:HB2	2.15	0.46
1:A:123:PHE:HA	5:A:606:HOH:O	2.15	0.46
1:A:188:ILE:HG23	1:A:278:HIS:CB	2.43	0.46
1:A:147:MET:HG2	1:A:231:VAL:HG21	1.98	0.46
1:A:191:ILE:O	1:A:194:GLU:N	2.45	0.45
1:A:152:ASP:HB3	1:A:154:THR:OG1	2.17	0.45
1:A:256:ARG:HA	1:A:257:PRO:HD3	1.82	0.45
1:A:222:GLY:HA3	1:A:225:LEU:HD13	1.98	0.44
1:A:292:LEU:O	1:A:296:GLU:HG2	2.17	0.44
1:A:186:THR:HG22	1:A:189:THR:HB	2.00	0.44
1:A:157:LEU:HD23	1:A:203:VAL:HG22	2.00	0.44
1:A:255:ARG:CG	1:A:255:ARG:CA	2.83	0.44
1:A:19:LEU:HD11	1:A:76:HIS:ND1	2.32	0.43
1:A:149:LEU:HB2	1:A:185:ARG:NH1	2.34	0.43
1:A:188:ILE:HG23	1:A:278:HIS:N	2.33	0.43
1:A:170:ILE:HG22	1:A:170:ILE:O	2.19	0.42
1:A:204:VAL:HG22	5:A:617:HOH:O	2.19	0.42
1:A:113:TYR:CD2	1:A:226:ASN:HB3	2.54	0.42
1:A:100:VAL:O	1:A:104:VAL:HG22	2.19	0.42
1:A:10:LYS:HZ2	1:A:57:LEU:HD11	1.84	0.42
1:A:159:ARG:HD3	1:A:280:CYS:SG	2.58	0.42
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.84	0.42
1:A:299:VAL:HG12	1:A:300:ASP:H	1.85	0.42
2:R:6:A:O2'	5:R:201:HOH:O	2.21	0.42
1:A:82:ILE:O	1:A:85:LEU:HB3	2.21	0.41
1:A:150:CYS:HA	1:A:181:VAL:CG1	2.51	0.41
1:A:49:PRO:HB3	1:A:57:LEU:HD21	2.03	0.41
1:A:13:LEU:HA	1:A:13:LEU:HD23	1.89	0.41
1:A:45:SER:HB2	1:A:51:ARG:NH2	2.36	0.41
1:A:220:LEU:HA	1:A:220:LEU:HD23	1.78	0.41
1:A:288:MET:O	1:A:292:LEU:HG	2.20	0.41
1:A:48:ASP:C	1:A:50:SER:N	2.61	0.40
1:A:78:ASN:HB3	1:A:237:PRO:HD3	2.04	0.40
1:A:106:HIS:CD2	1:A:107:PRO:HD2	2.56	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	283/409 (69%)	274 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	256/373 (69%)	228 (89%)	28 (11%)	6	21

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	22	SER
1	A	26	ARG
1	A	51	ARG
1	A	54	HIS
1	A	69	ASP
1	A	80	LEU
1	A	82	ILE
1	A	84	ASN
1	A	89	SER
1	A	103	THR
1	A	121	ASP
1	A	127	VAL

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Mol	Chain	Res	Type
1	A	130	LYS
1	A	141	VAL
1	A	150	CYS
1	A	160	VAL
1	A	166	ASP
1	A	169	VAL
1	A	171	LEU
1	A	181	VAL
1	A	182	VAL
1	A	189	THR
1	A	206	ILE
1	A	246	PHE
1	A	255	ARG
1	A	276	VAL
1	A	299	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	8/10 (80%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	SO4	R	101	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	A	501	-	4,4,4	0.26	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	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 [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	288/409 (70%)	0.25	18 (6%) 26 19	45, 100, 146, 193	1 (0%)
2	R	9/10 (90%)	-0.00	0 100 100	102, 107, 157, 171	0
All	All	297/419 (70%)	0.24	18 (6%) 27 20	45, 101, 148, 193	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	300	ASP	4.9
1	A	44	ASP	3.9
1	A	33	LYS	3.7
1	A	196	ILE	3.5
1	A	275	GLY	3.2
1	A	255	ARG	3.1
1	A	193	ALA	2.9
1	A	42	ASN	2.8
1	A	295	VAL	2.8
1	A	35	PHE	2.8
1	A	195	ASP	2.5
1	A	39	TYR	2.4
1	A	199	ALA	2.3
1	A	156	GLY	2.3
1	A	198	ASN	2.2
1	A	276	VAL	2.2
1	A	265	SER	2.1
1	A	278	HIS	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($\text{\AA}^2$)	Q<0.9
3	SO4	R	101	5/5	0.68	0.10	150,152,157,171	0
4	MG	A	503	1/1	0.86	0.10	108,108,108,108	1
4	MG	A	502	1/1	0.91	0.47	81,81,81,81	0
3	SO4	A	501	5/5	0.91	0.10	134,136,139,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.