



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:50 AM UTC

PDB ID : 3EF9 / pdb_00003ef9
Title : Replacement of Val3 in Human Thymidylate Synthase Affects Its Kinetic Properties and Intracellular Stability
Authors : Huang, X.; Gibson, L.M.; Bell, B.J.; Lovelace, L.L.; Pena, M.M.; Berger, F.G.; Berger, S.H.
Deposited on : 2008-09-08
Resolution : 3.20 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

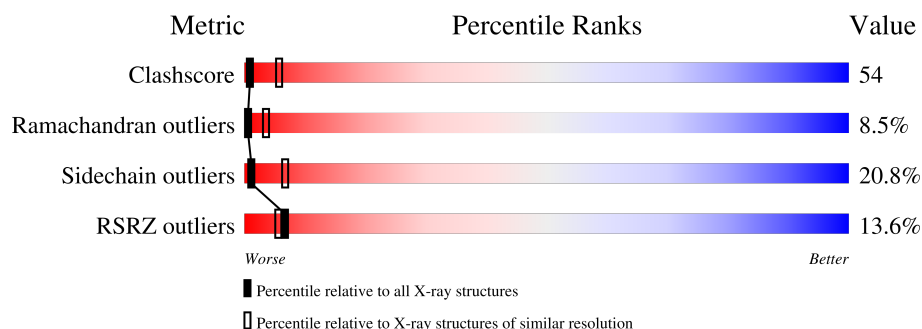
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	313	

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	317	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2171 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.

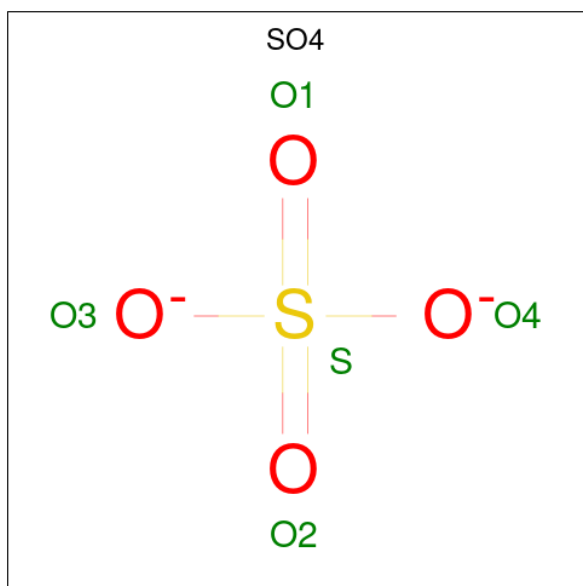
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	264	2134	1368	373	381	12	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	LEU	VAL	engineered mutation	UNP P04818

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	27	Total	O	0	0
			27	27		

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	96.35Å 96.35Å 83.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 50.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	74.2 (50.00-3.20) 74.2 (50.00-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-1.05 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.252 , 0.298 0.251 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 110.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.065 for -h,-k,l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	2171	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.70	6/2189 (0.3%)	1.14	14/2959 (0.5%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	ARG	CA-CB	9.79	1.65	1.53
1	A	26	PRO	C-O	9.20	1.42	1.23
1	A	27	PRO	N-CA	8.26	1.61	1.47
1	A	43	CYS	CA-C	-6.72	1.43	1.52
1	A	28	HIS	N-CA	5.82	1.53	1.45
1	A	274	ARG	NE-CZ	5.06	1.38	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	PRO	O-C-N	-9.70	107.47	123.00
1	A	42	ARG	N-CA-C	9.42	125.27	107.75
1	A	41	LEU	CA-C-N	-9.14	110.14	122.85
1	A	41	LEU	C-N-CA	-9.14	110.14	122.85
1	A	26	PRO	C-N-CD	-8.83	101.18	120.60
1	A	42	ARG	CA-C-O	7.76	129.23	120.84
1	A	274	ARG	NE-CZ-NH2	-7.31	112.62	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLY	N-CA-C	-6.79	100.39	112.54
1	A	27	PRO	N-CA-C	6.24	128.31	112.10
1	A	26	PRO	CA-C-N	5.89	141.13	127.00
1	A	26	PRO	C-N-CA	5.89	141.13	127.00
1	A	59	PHE	N-CA-C	5.61	117.88	108.23
1	A	183	ASN	CA-C-N	5.32	126.49	119.84
1	A	183	ASN	C-N-CA	5.32	126.49	119.84

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	PRO	Mainchain
1	A	274	ARG	Sidechain
1	A	42	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	2134	0	2123	232	0
2	A	10	0	0	0	0
3	A	27	0	0	1	0
All	All	2171	0	2123	232	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 54.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD21	1:A:213:TYR:HB3	1.18	1.17
1:A:42:ARG:O	1:A:42:ARG:CD	1.99	1.11
1:A:42:ARG:O	1:A:42:ARG:HD3	1.58	1.01
1:A:34:LEU:HA	1:A:37:ILE:HD12	1.44	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:CD2	1:A:213:TYR:HB3	1.92	0.97
1:A:77:LYS:HB2	1:A:307:ILE:HD13	1.46	0.95
1:A:67:LEU:HD21	1:A:248:PHE:HB2	1.51	0.93
1:A:283:ARG:HH22	1:A:292:LYS:HG3	1.33	0.91
1:A:161:LEU:HG	1:A:165:ILE:HD11	1.57	0.86
1:A:42:ARG:O	1:A:42:ARG:HD2	1.76	0.83
1:A:57:SER:HB3	1:A:256:HIS:HB3	1.61	0.82
1:A:201:PHE:HD1	1:A:208:LEU:HD11	1.44	0.81
1:A:28:HIS:HB3	1:A:31:LEU:HD23	1.62	0.81
1:A:36:GLN:O	1:A:40:ILE:HD12	1.80	0.81
1:A:211:GLN:HG3	1:A:249:ILE:HB	1.62	0.79
1:A:106:VAL:O	1:A:107:LYS:HD3	1.83	0.79
1:A:33:TYR:CE1	1:A:37:ILE:HD11	2.19	0.78
1:A:42:ARG:CD	1:A:42:ARG:C	2.57	0.78
1:A:82:LYS:HE2	1:A:82:LYS:H	1.48	0.77
1:A:46:ARG:HG3	1:A:56:LEU:HD11	1.66	0.77
1:A:40:ILE:HG21	1:A:257:ILE:HG12	1.66	0.76
1:A:46:ARG:H	1:A:46:ARG:HD2	1.51	0.75
1:A:82:LYS:O	1:A:86:GLU:HB2	1.87	0.75
1:A:55:THR:HG22	1:A:258:TYR:HA	1.70	0.74
1:A:88:LEU:HD23	1:A:232:LEU:HD23	1.68	0.74
1:A:40:ILE:HD11	1:A:219:MET:HE2	1.72	0.71
1:A:204:VAL:HG22	1:A:205:ASN:HD22	1.55	0.70
1:A:232:LEU:HG	1:A:236:MET:HE3	1.74	0.70
1:A:271:ARG:HB3	1:A:304:HIS:ND1	2.07	0.70
1:A:81:TRP:HH2	1:A:232:LEU:HD13	1.57	0.69
1:A:26:PRO:HD2	1:A:27:PRO:O	1.92	0.69
1:A:30:GLU:HG3	1:A:74:LEU:HD13	1.73	0.69
1:A:74:LEU:HD23	1:A:74:LEU:H	1.58	0.68
1:A:287:LYS:HD3	1:A:289:ASP:H	1.58	0.68
1:A:31:LEU:HD22	1:A:273:PRO:HG2	1.77	0.67
1:A:271:ARG:HH21	1:A:304:HIS:HB3	1.58	0.67
1:A:153:TYR:HA	1:A:156:GLN:NE2	2.09	0.67
1:A:282:LEU:HD11	1:A:295:ASP:HA	1.77	0.67
1:A:240:ILE:HG22	1:A:286:GLU:HA	1.77	0.66
1:A:201:PHE:CE1	1:A:237:ILE:HD12	2.31	0.65
1:A:232:LEU:O	1:A:236:MET:HG3	1.96	0.65
1:A:209:SER:HB3	1:A:247:ASP:H	1.62	0.65
1:A:73:LEU:HD11	1:A:79:VAL:HB	1.78	0.65
1:A:221:LEU:HD23	1:A:309:MET:HB2	1.78	0.65
1:A:265:LEU:HD21	1:A:309:MET:HE1	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PRO:O	1:A:184:PRO:HG3	1.97	0.64
1:A:42:ARG:HD3	1:A:43:CYS:HB2	1.78	0.64
1:A:99:LYS:HA	1:A:102:SER:OG	1.98	0.63
1:A:261:HIS:O	1:A:264:PRO:HD2	2.00	0.62
1:A:80:PHE:CD1	1:A:82:LYS:HE3	2.35	0.62
1:A:258:TYR:O	1:A:261:HIS:HB2	2.00	0.61
1:A:91:PHE:CE1	1:A:135:TYR:HB2	2.35	0.61
1:A:33:TYR:CD1	1:A:37:ILE:HD11	2.36	0.61
1:A:82:LYS:H	1:A:82:LYS:CE	2.13	0.61
1:A:97:ASN:HD21	1:A:99:LYS:HB3	1.66	0.60
1:A:29:GLY:O	1:A:32:GLN:HB2	2.02	0.60
1:A:30:GLU:CD	1:A:74:LEU:HD13	2.26	0.60
1:A:50:ARG:HH11	1:A:185:ARG:CZ	2.14	0.60
1:A:49:ASP:OD1	1:A:51:THR:HG23	2.01	0.60
1:A:244:LYS:HZ3	1:A:244:LYS:HB2	1.66	0.60
1:A:46:ARG:HA	1:A:55:THR:O	2.02	0.59
1:A:30:GLU:HG2	1:A:34:LEU:HD21	1.84	0.59
1:A:74:LEU:HD23	1:A:74:LEU:N	2.15	0.59
1:A:85:LEU:HD11	1:A:296:PHE:CD1	2.37	0.59
1:A:186:ASP:HA	1:A:189:LEU:HB2	1.83	0.59
1:A:30:GLU:CG	1:A:74:LEU:HD13	2.33	0.59
1:A:208:LEU:HB2	1:A:243:LEU:HD13	1.84	0.59
1:A:187:LEU:HB2	1:A:188:PRO:HD3	1.85	0.58
1:A:236:MET:HE2	1:A:296:PHE:CZ	2.38	0.57
1:A:77:LYS:HZ3	1:A:309:MET:HE3	1.69	0.57
1:A:90:TRP:CH2	1:A:134:VAL:HG21	2.39	0.57
1:A:306:THR:C	1:A:307:ILE:HD12	2.29	0.57
1:A:177:ILE:HD12	1:A:201:PHE:O	2.05	0.57
1:A:161:LEU:O	1:A:165:ILE:HG12	2.04	0.57
1:A:57:SER:HB2	1:A:254:ASP:OD2	2.05	0.57
1:A:81:TRP:N	1:A:82:LYS:HE2	2.20	0.56
1:A:283:ARG:HG2	1:A:284:LYS:N	2.21	0.56
1:A:177:ILE:HD12	1:A:201:PHE:C	2.31	0.56
1:A:182:TRP:CD1	1:A:195:CYS:HA	2.41	0.56
1:A:258:TYR:HB2	1:A:261:HIS:ND1	2.21	0.56
1:A:261:HIS:NE2	1:A:309:MET:HB3	2.21	0.56
1:A:208:LEU:HD23	1:A:238:ALA:HB2	1.89	0.55
1:A:261:HIS:HE2	1:A:309:MET:HB3	1.70	0.55
1:A:36:GLN:O	1:A:39:HIS:HB3	2.07	0.55
1:A:237:ILE:O	1:A:241:THR:HG23	2.07	0.55
1:A:287:LYS:HE2	1:A:288:ILE:HG22	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:HG2	1:A:284:LYS:H	1.70	0.55
1:A:32:GLN:O	1:A:36:GLN:HG3	2.06	0.54
1:A:96:THR:O	1:A:131:LEU:HD11	2.07	0.54
1:A:261:HIS:CD2	1:A:309:MET:HB3	2.43	0.54
1:A:96:THR:O	1:A:131:LEU:HD21	2.06	0.54
1:A:42:ARG:O	1:A:43:CYS:HB2	2.07	0.54
1:A:34:LEU:HD11	1:A:273:PRO:HG3	1.90	0.54
1:A:244:LYS:HB2	1:A:244:LYS:NZ	2.22	0.53
1:A:261:HIS:CE1	1:A:310:GLU:HG2	2.44	0.53
1:A:302:ASN:HB2	3:A:328:HOH:O	2.08	0.53
1:A:175:ARG:O	1:A:177:ILE:HG13	2.09	0.53
1:A:184:PRO:HA	1:A:187:LEU:CD1	2.39	0.53
1:A:279:LEU:HD12	1:A:280:ARG:N	2.24	0.52
1:A:137:PHE:CE2	1:A:141:HIS:HB2	2.44	0.52
1:A:205:ASN:O	1:A:206:SER:HB2	2.10	0.52
1:A:207:GLU:HG3	1:A:244:LYS:NZ	2.24	0.52
1:A:198:LEU:O	1:A:198:LEU:HD23	2.08	0.52
1:A:204:VAL:HG22	1:A:205:ASN:ND2	2.22	0.52
1:A:201:PHE:CD1	1:A:208:LEU:HD11	2.35	0.52
1:A:232:LEU:HD11	1:A:296:PHE:CE2	2.44	0.52
1:A:249:ILE:HD12	1:A:249:ILE:N	2.24	0.52
1:A:81:TRP:CH2	1:A:232:LEU:HD13	2.43	0.52
1:A:82:LYS:HE2	1:A:82:LYS:N	2.23	0.51
1:A:153:TYR:HD2	1:A:156:GLN:OE1	1.93	0.51
1:A:282:LEU:CD1	1:A:295:ASP:HA	2.39	0.51
1:A:73:LEU:HB3	1:A:277:PRO:HG2	1.93	0.51
1:A:282:LEU:O	1:A:283:ARG:HB2	2.12	0.50
1:A:46:ARG:HG3	1:A:56:LEU:CD1	2.38	0.50
1:A:263:GLU:HB2	1:A:264:PRO:HD3	1.93	0.50
1:A:207:GLU:HG3	1:A:244:LYS:HZ2	1.77	0.49
1:A:68:ARG:HG3	1:A:68:ARG:HH11	1.77	0.49
1:A:219:MET:HB2	1:A:257:ILE:HD13	1.94	0.49
1:A:223:VAL:HB	1:A:224:PRO:HD3	1.94	0.49
1:A:101:LEU:O	1:A:106:VAL:CG2	2.61	0.49
1:A:66:SER:O	1:A:70:GLU:OE1	2.31	0.49
1:A:82:LYS:H	1:A:82:LYS:CD	2.25	0.49
1:A:159:ASP:CG	1:A:162:GLN:HB2	2.38	0.49
1:A:283:ARG:HH22	1:A:292:LYS:CG	2.17	0.49
1:A:64:ARG:HA	1:A:248:PHE:O	2.12	0.48
1:A:276:PHE:HD1	1:A:277:PRO:HD2	1.78	0.48
1:A:130:ASP:OD1	1:A:146:TYR:OH	2.30	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PRO:O	1:A:138:GLN:OE1	2.31	0.48
1:A:37:ILE:HA	1:A:40:ILE:HD13	1.95	0.48
1:A:153:TYR:HB3	1:A:156:GLN:HB2	1.94	0.48
1:A:201:PHE:HE1	1:A:237:ILE:HD12	1.75	0.48
1:A:248:PHE:C	1:A:249:ILE:HD12	2.39	0.48
1:A:251:THR:O	1:A:252:LEU:HD13	2.14	0.48
1:A:31:LEU:CD2	1:A:273:PRO:HG2	2.42	0.48
1:A:30:GLU:O	1:A:34:LEU:HG	2.13	0.48
1:A:276:PHE:CD1	1:A:277:PRO:HD2	2.49	0.48
1:A:240:ILE:HG22	1:A:286:GLU:CA	2.42	0.48
1:A:134:VAL:O	1:A:138:GLN:OE1	2.31	0.48
1:A:184:PRO:HA	1:A:187:LEU:HD11	1.95	0.48
1:A:279:LEU:HD12	1:A:280:ARG:H	1.78	0.48
1:A:282:LEU:HD11	1:A:294:GLU:O	2.13	0.48
1:A:74:LEU:HA	1:A:276:PHE:HE1	1.79	0.47
1:A:59:PHE:HD2	1:A:253:GLY:O	1.97	0.47
1:A:265:LEU:CD2	1:A:309:MET:HE1	2.44	0.47
1:A:26:PRO:CD	1:A:27:PRO:O	2.61	0.47
1:A:67:LEU:CD2	1:A:248:PHE:HB2	2.34	0.47
1:A:211:GLN:HG3	1:A:249:ILE:CB	2.39	0.47
1:A:307:ILE:HG22	1:A:307:ILE:O	2.14	0.47
1:A:28:HIS:HB3	1:A:31:LEU:CD2	2.41	0.47
1:A:38:GLN:OE1	1:A:269:LEU:HD13	2.16	0.46
1:A:284:LYS:HD3	1:A:286:GLU:OE1	2.15	0.46
1:A:197:ALA:O	1:A:198:LEU:HB3	2.13	0.46
1:A:203:VAL:HA	1:A:207:GLU:O	2.14	0.46
1:A:263:GLU:HA	1:A:266:LYS:HG3	1.98	0.46
1:A:281:ILE:N	1:A:281:ILE:HD12	2.31	0.46
1:A:57:SER:HB2	1:A:255:ALA:O	2.16	0.46
1:A:36:GLN:C	1:A:40:ILE:HD12	2.39	0.45
1:A:178:ILE:HG22	1:A:179:MET:N	2.31	0.45
1:A:166:ASP:O	1:A:170:THR:HG23	2.16	0.45
1:A:57:SER:CB	1:A:256:HIS:HB3	2.41	0.45
1:A:96:THR:HG23	1:A:137:PHE:HB2	1.97	0.45
1:A:40:ILE:HG21	1:A:257:ILE:CG1	2.42	0.45
1:A:140:ARG:NH1	1:A:289:ASP:OD2	2.50	0.45
1:A:236:MET:HE2	1:A:296:PHE:HZ	1.81	0.45
1:A:87:GLU:HG2	1:A:91:PHE:CZ	2.52	0.45
1:A:153:TYR:O	1:A:156:GLN:N	2.49	0.45
1:A:49:ASP:OD1	1:A:51:THR:N	2.50	0.45
1:A:63:ALA:O	1:A:249:ILE:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:VAL:O	1:A:227:ILE:HG12	2.17	0.45
1:A:262:ILE:HG22	1:A:263:GLU:N	2.31	0.45
1:A:101:LEU:O	1:A:106:VAL:HG23	2.17	0.45
1:A:226:ASN:HA	1:A:229:SER:HB2	1.98	0.44
1:A:42:ARG:HD3	1:A:42:ARG:C	2.31	0.44
1:A:104:LYS:HB3	1:A:104:LYS:HE2	1.57	0.44
1:A:131:LEU:HD12	1:A:134:VAL:HG13	1.99	0.44
1:A:240:ILE:HD11	1:A:288:ILE:HD13	1.98	0.44
1:A:257:ILE:HD12	1:A:265:LEU:CD1	2.48	0.44
1:A:30:GLU:OE1	1:A:74:LEU:HD13	2.16	0.44
1:A:178:ILE:HA	1:A:200:GLN:HA	2.00	0.44
1:A:259:LEU:HA	1:A:262:ILE:HD13	1.99	0.44
1:A:30:GLU:CD	1:A:76:THR:HG23	2.43	0.44
1:A:153:TYR:O	1:A:155:GLY:N	2.51	0.44
1:A:164:VAL:HG21	1:A:179:MET:HE2	1.99	0.44
1:A:217:GLY:O	1:A:256:HIS:ND1	2.51	0.44
1:A:212:LEU:HD22	1:A:230:TYR:CD2	2.53	0.44
1:A:34:LEU:N	1:A:34:LEU:HD23	2.33	0.43
1:A:134:VAL:HG23	1:A:136:GLY:H	1.84	0.43
1:A:158:VAL:O	1:A:158:VAL:HG12	2.18	0.43
1:A:258:TYR:O	1:A:261:HIS:N	2.49	0.43
1:A:182:TRP:NE1	1:A:195:CYS:HA	2.34	0.43
1:A:271:ARG:CZ	1:A:307:ILE:HD11	2.49	0.43
1:A:211:GLN:CG	1:A:249:ILE:HB	2.40	0.43
1:A:292:LYS:HE2	1:A:292:LYS:HB3	1.53	0.43
1:A:32:GLN:HE22	1:A:64:ARG:C	2.25	0.43
1:A:33:TYR:CZ	1:A:37:ILE:HD11	2.54	0.43
1:A:283:ARG:NH2	1:A:295:ASP:OD1	2.51	0.43
1:A:85:LEU:HD11	1:A:296:PHE:CG	2.53	0.43
1:A:137:PHE:CZ	1:A:146:TYR:HB2	2.54	0.43
1:A:50:ARG:HD2	1:A:185:ARG:NH1	2.34	0.43
1:A:189:LEU:HD22	1:A:189:LEU:HA	1.75	0.43
1:A:93:LYS:O	1:A:93:LYS:HG3	2.18	0.42
1:A:271:ARG:NH2	1:A:304:HIS:HB3	2.28	0.42
1:A:73:LEU:O	1:A:74:LEU:O	2.36	0.42
1:A:178:ILE:HG22	1:A:179:MET:H	1.84	0.42
1:A:309:MET:O	1:A:310:GLU:HG3	2.20	0.42
1:A:34:LEU:HD11	1:A:76:THR:HG21	2.01	0.42
1:A:176:ARG:H	1:A:176:ARG:HG3	1.52	0.42
1:A:73:LEU:O	1:A:73:LEU:HG	2.20	0.42
1:A:212:LEU:HD12	1:A:213:TYR:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LYS:HB2	1:A:295:ASP:OD1	2.20	0.42
1:A:71:PHE:CD2	1:A:72:PRO:HD2	2.54	0.42
1:A:306:THR:O	1:A:307:ILE:HD12	2.20	0.41
1:A:206:SER:HB3	1:A:244:LYS:HD3	2.03	0.41
1:A:77:LYS:HG3	1:A:78:ARG:N	2.34	0.41
1:A:237:ILE:O	1:A:240:ILE:HG13	2.21	0.41
1:A:55:THR:HB	1:A:257:ILE:O	2.21	0.41
1:A:241:THR:OG1	1:A:243:LEU:HD12	2.21	0.41
1:A:99:LYS:O	1:A:103:SER:HB3	2.21	0.41
1:A:148:ASP:OD1	1:A:150:GLU:N	2.53	0.41
1:A:226:ASN:O	1:A:229:SER:HB2	2.21	0.41
1:A:75:THR:C	1:A:77:LYS:H	2.29	0.41
1:A:174:ASP:OD1	1:A:175:ARG:N	2.53	0.41
1:A:261:HIS:HE1	1:A:310:GLU:HG2	1.84	0.41
1:A:88:LEU:CD2	1:A:232:LEU:HD23	2.45	0.40
1:A:34:LEU:CA	1:A:37:ILE:HD12	2.32	0.40
1:A:236:MET:HB3	1:A:291:PHE:CE2	2.56	0.40
1:A:244:LYS:HA	1:A:245:PRO:HD3	1.86	0.40
1:A:32:GLN:NE2	1:A:64:ARG:O	2.53	0.40
1:A:40:ILE:CD1	1:A:219:MET:HE2	2.47	0.40
1:A:261:HIS:C	1:A:264:PRO:HD2	2.46	0.40
1:A:219:MET:HB2	1:A:257:ILE:CD1	2.51	0.40
1:A:261:HIS:HD2	1:A:309:MET:SD	2.45	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	260/313 (83%)	197 (76%)	41 (16%)	22 (8%)	0 3

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	CYS
1	A	74	LEU
1	A	134	VAL
1	A	77	LYS
1	A	86	GLU
1	A	131	LEU
1	A	154	SER
1	A	159	ASP
1	A	176	ARG
1	A	198	LEU
1	A	282	LEU
1	A	220	GLY
1	A	291	PHE
1	A	306	THR
1	A	27	PRO
1	A	137	PHE
1	A	229	SER
1	A	307	ILE
1	A	227	ILE
1	A	305	PRO
1	A	262	ILE
1	A	277	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	231/271 (85%)	183 (79%)	48 (21%)	1 7

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	36	GLN
1	A	42	ARG
1	A	43	CYS
1	A	45	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	47	LYS
1	A	51	THR
1	A	58	VAL
1	A	61	MET
1	A	67	LEU
1	A	74	LEU
1	A	77	LYS
1	A	80	PHE
1	A	82	LYS
1	A	86	GLU
1	A	99	LYS
1	A	104	LYS
1	A	106	VAL
1	A	131	LEU
1	A	138	GLN
1	A	149	MET
1	A	150	GLU
1	A	154	SER
1	A	165	ILE
1	A	175	ARG
1	A	177	ILE
1	A	189	LEU
1	A	192	LEU
1	A	199	CYS
1	A	209	SER
1	A	221	LEU
1	A	229	SER
1	A	235	TYR
1	A	240	ILE
1	A	244	LYS
1	A	252	LEU
1	A	257	ILE
1	A	259	LEU
1	A	266	LYS
1	A	278	LYS
1	A	282	LEU
1	A	284	LYS
1	A	285	VAL
1	A	287	LYS
1	A	292	LYS
1	A	294	GLU
1	A	309	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	310	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	ASN
1	A	160	GLN
1	A	171	ASN
1	A	183	ASN
1	A	205	ASN
1	A	226	ASN
1	A	261	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	317	-	4,4,4	1.31	0	6,6,6	5.28	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	316	-	4,4,4	0.83	0	6,6,6	3.09	3 (50%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	317	SO4	O2-S-O1	-8.07	52.18	109.06
2	A	317	SO4	O3-S-O2	7.37	148.07	109.56
2	A	316	SO4	O4-S-O1	-5.51	80.77	109.56
2	A	317	SO4	O4-S-O1	4.96	135.48	109.56
2	A	317	SO4	O4-S-O2	-4.77	84.63	109.56
2	A	316	SO4	O4-S-O2	-4.16	87.79	109.56
2	A	316	SO4	O2-S-O1	2.11	123.95	109.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	264/313 (84%)	0.89	36 (13%) 7 5	15, 57, 172, 172	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PRO	6.5
1	A	101	LEU	5.6
1	A	135	TYR	5.1
1	A	103	SER	4.8
1	A	50	ARG	4.5
1	A	100	GLU	4.1
1	A	196	HIS	3.6
1	A	98	ALA	3.6
1	A	43	CYS	3.5
1	A	134	VAL	3.4
1	A	92	ILE	3.2
1	A	131	LEU	3.1
1	A	136	GLY	3.1
1	A	104	LYS	3.0
1	A	139	TRP	2.9
1	A	132	GLY	2.8
1	A	190	MET	2.7
1	A	138	GLN	2.7
1	A	105	GLY	2.7
1	A	193	PRO	2.6
1	A	142	PHE	2.5
1	A	102	SER	2.4
1	A	106	VAL	2.4
1	A	95	SER	2.4
1	A	302	ASN	2.4
1	A	146	TYR	2.4
1	A	192	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	26	PRO	2.4
1	A	96	THR	2.3
1	A	42	ARG	2.3
1	A	158	VAL	2.2
1	A	194	PRO	2.2
1	A	141	HIS	2.2
1	A	87	GLU	2.2
1	A	140	ARG	2.2
1	A	129	GLY	2.1

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
2	SO4	A	317	5/5	0.82	0.17	47,49,61,68	0
2	SO4	A	316	5/5	0.88	0.12	45,46,56,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.