



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:10 PM UTC

PDB ID : 1E2J / pdb_00001e2j
Title : The nucleoside binding site of Herpes simplex type 1 thymidine kinase analyzed by X-ray crystallography
Authors : Vogt, J.; Scapozza, L.; Schulz, G.E.
Deposited on : 2000-05-23
Resolution : 2.50 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

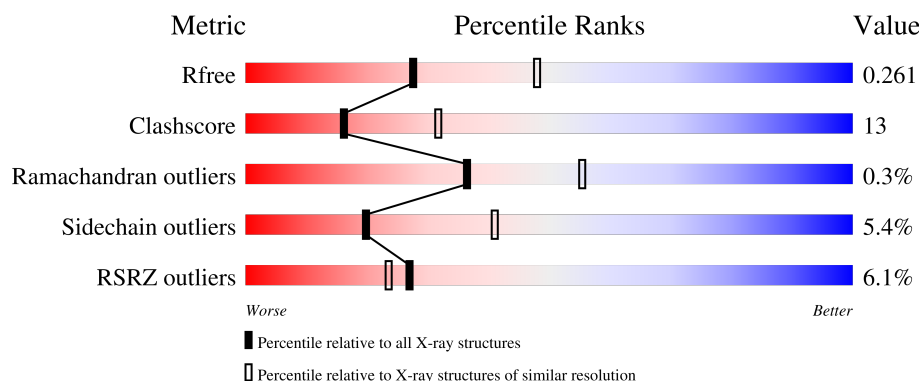
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	331	
1	B	331	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4884 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.

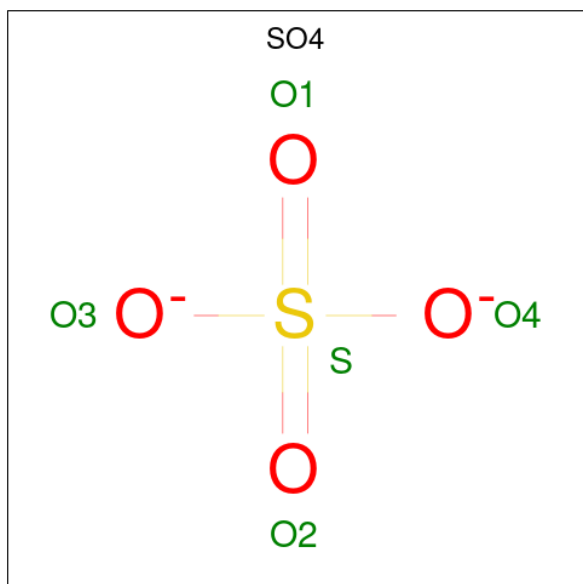
- Molecule 1 is a protein called THYMIDINE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2346	1494	411	425	16			
1	B	314	Total	C	N	O	S	0	0	0
			2383	1518	414	435	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	ASN	GLN	engineered mutation	UNP P03176
B	125	ASN	GLN	engineered mutation	UNP P03176

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



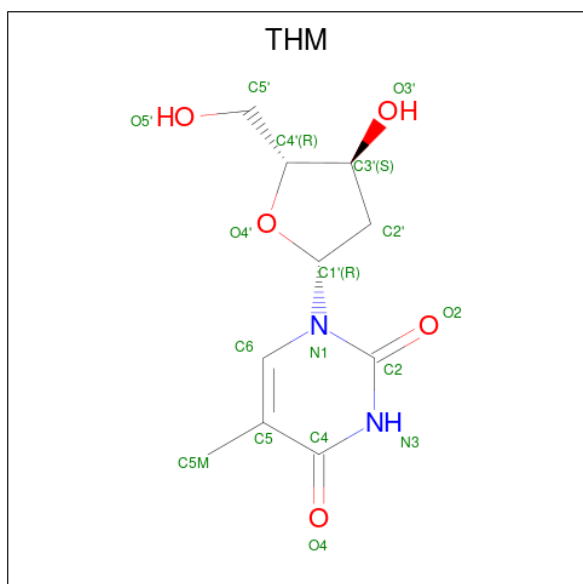
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is THYMIDINE (CCD ID: THM) (formula: $C_{10}H_{14}N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	10	2	5		
3	B	1	Total	C	N	O	0	0
			17	10	2	5		

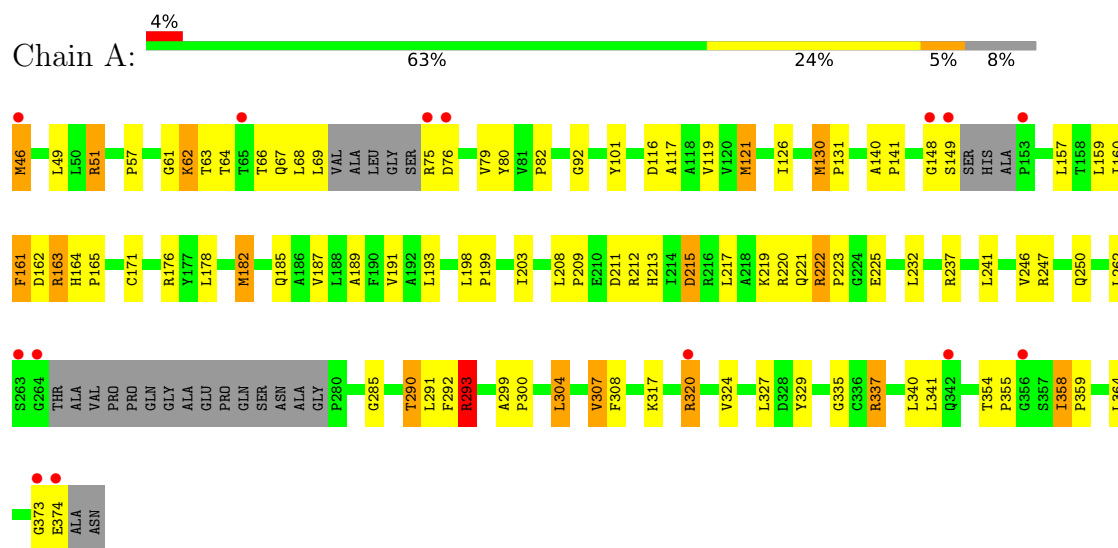
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	54	Total	O	0	0
			54	54		

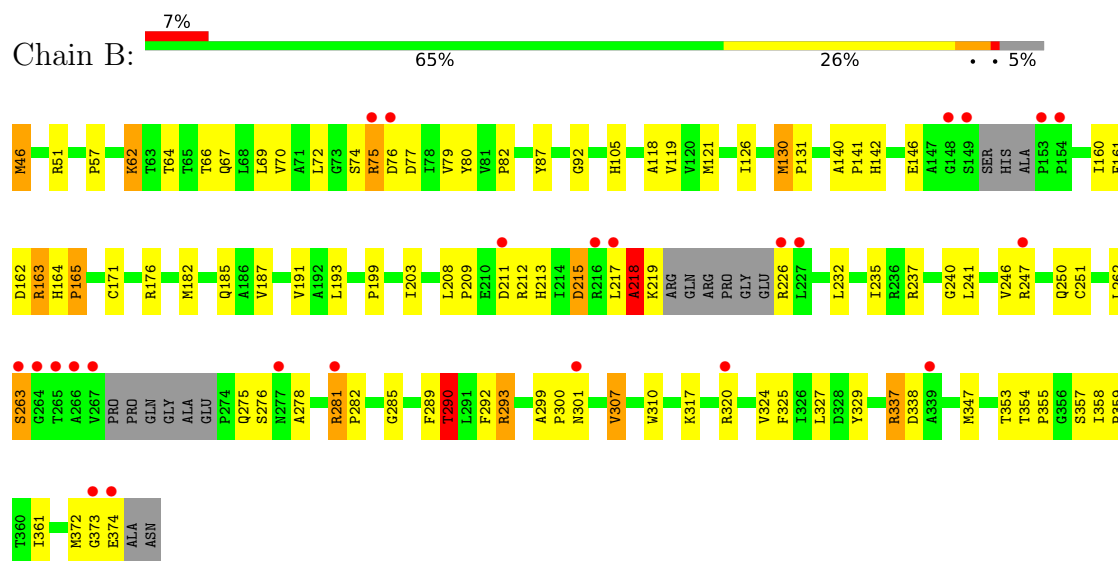
3 Residue-property plots [i](#)

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: THYMIDINE KINASE



• Molecule 1: THYMIDINE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.40Å 117.50Å 108.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.50) 91.3 (20.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.38 (at 2.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.273 0.208 , 0.261	Depositor DCC
R_{free} test set	1247 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.030 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4884	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 6.03% 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: THM, 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	0.62	0/2400	1.34	15/3272 (0.5%)
1	B	0.60	0/2437	1.36	23/3326 (0.7%)
All	All	0.61	0/4837	1.35	38/6598 (0.6%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	ARG	CD-NE-CZ	12.00	141.21	124.40
1	A	222	ARG	CD-NE-CZ	11.77	140.88	124.40
1	B	51	ARG	CD-NE-CZ	9.64	137.89	124.40
1	B	292	PHE	CA-CB-CG	-8.55	105.25	113.80
1	B	337	ARG	CA-C-N	7.63	130.51	120.28
1	B	337	ARG	C-N-CA	7.63	130.51	120.28
1	B	163	ARG	NE-CZ-NH2	7.53	125.98	119.20
1	A	292	PHE	CA-CB-CG	-7.52	106.28	113.80
1	A	163	ARG	NH1-CZ-NH2	-6.62	110.69	119.30
1	A	171	CYS	N-CA-C	6.50	118.05	110.97
1	A	320	ARG	CG-CD-NE	6.47	126.24	112.00
1	A	116	ASP	CA-CB-CG	6.29	118.89	112.60
1	B	240	GLY	N-CA-C	-6.08	105.45	112.50
1	B	76	ASP	N-CA-C	6.04	120.78	113.17
1	A	161	PHE	CA-CB-CG	6.03	119.83	113.80
1	B	293	ARG	CD-NE-CZ	6.02	132.83	124.40
1	A	307	VAL	CB-CA-C	-6.01	104.19	111.88
1	B	338	ASP	N-CA-C	-5.97	104.77	111.28
1	B	163	ARG	NH1-CZ-NH2	-5.96	111.56	119.30
1	B	161	PHE	CA-CB-CG	5.95	119.75	113.80
1	B	301	ASN	CA-CB-CG	5.88	118.48	112.60
1	A	337	ARG	CD-NE-CZ	5.80	132.53	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ARG	N-CA-C	-5.77	106.14	112.72
1	B	171	CYS	N-CA-C	5.67	117.14	110.97
1	B	290	THR	CB-CA-C	-5.67	101.39	110.79
1	A	358	ILE	CA-C-N	5.55	125.21	119.05
1	A	358	ILE	C-N-CA	5.55	125.21	119.05
1	A	76	ASP	N-CA-C	5.54	120.15	113.17
1	A	335	GLY	N-CA-C	-5.52	106.10	112.50
1	B	67	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	B	289	PHE	CA-CB-CG	-5.37	108.43	113.80
1	B	372	MET	N-CA-C	5.17	120.24	113.88
1	B	218	ALA	CA-C-N	5.17	131.00	121.70
1	B	218	ALA	C-N-CA	5.17	131.00	121.70
1	B	307	VAL	CB-CA-C	-5.16	105.27	111.88
1	B	64	THR	CA-C-N	5.11	127.44	120.54
1	B	64	THR	C-N-CA	5.11	127.44	120.54
1	B	281	ARG	CA-C-O	5.02	124.23	119.76

There are no chirality outliers.

There are no planarity outliers.

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	2346	0	2362	63	0
1	B	2383	0	2400	68	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	17	0	14	0	0
3	B	17	0	14	0	0
4	A	57	0	0	2	0
4	B	54	0	0	2	0
All	All	4884	0	4790	125	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 13.

All (125) 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:119:VAL:HG12	1:B:119:VAL:HG12	1.48	0.95
1:B:66:THR:HG23	1:B:160:ILE:HG21	1.58	0.85
1:B:130:MET:HB3	1:B:131:PRO:HD3	1.60	0.83
1:A:358:ILE:HB	1:A:359:PRO:HD3	1.60	0.83
1:B:358:ILE:HB	1:B:359:PRO:HD3	1.63	0.80
1:B:285:GLY:HA2	1:B:290:THR:HG23	1.67	0.76
1:A:69:LEU:HD23	1:A:340:LEU:HD23	1.66	0.76
1:B:246:VAL:HG21	1:B:324:VAL:HG21	1.69	0.75
1:A:285:GLY:HA2	1:A:290:THR:HG23	1.70	0.73
1:B:121:MET:HE3	1:B:176:ARG:HD2	1.73	0.71
1:B:75:ARG:HE	1:B:75:ARG:H	1.39	0.70
1:B:70:VAL:HG21	1:B:80:TYR:HB2	1.74	0.70
1:B:217:LEU:HD22	1:B:232:LEU:HD13	1.74	0.69
1:B:66:THR:HG21	1:B:80:TYR:CE1	2.27	0.69
1:A:130:MET:HB3	1:A:131:PRO:HD3	1.75	0.69
1:B:140:ALA:HB3	1:B:141:PRO:HD3	1.78	0.66
1:A:217:LEU:HD22	1:A:232:LEU:HD13	1.80	0.63
1:B:354:THR:HB	1:B:355:PRO:HD2	1.82	0.62
1:A:121:MET:HE3	1:A:176:ARG:HD2	1.81	0.61
1:A:69:LEU:HB2	1:A:337:ARG:HG2	1.83	0.60
1:A:64:THR:O	1:A:68:LEU:HG	2.01	0.60
1:B:105:HIS:CG	1:B:226:ARG:HH11	2.20	0.59
1:B:262:LEU:O	1:B:263:SER:C	2.45	0.59
1:B:187:VAL:O	1:B:191:VAL:HG23	2.02	0.59
1:A:92:GLY:HA2	1:B:185:GLN:HG2	1.84	0.59
1:B:275:GLN:NE2	1:B:278:ALA:HB3	2.19	0.58
1:A:51:ARG:HG3	4:A:2002:HOH:O	2.02	0.58
1:A:62:LYS:NZ	1:A:62:LYS:HB2	2.19	0.58
1:A:61:GLY:HA2	1:A:220:ARG:HH11	1.69	0.57
1:B:62:LYS:HB2	1:B:62:LYS:NZ	2.21	0.56
1:A:354:THR:HB	1:A:355:PRO:HD2	1.87	0.56
1:A:246:VAL:HG21	1:A:324:VAL:HG21	1.88	0.56
1:B:276:SER:HB2	1:B:324:VAL:HB	1.88	0.55
1:A:185:GLN:HG2	1:B:92:GLY:HA2	1.88	0.55
1:B:246:VAL:O	1:B:250:GLN:HG3	2.06	0.55
1:B:299:ALA:HB1	1:B:300:PRO:HD2	1.88	0.55
1:B:218:ALA:O	1:B:219:LYS:HB2	2.08	0.54
1:B:130:MET:HB3	1:B:131:PRO:CD	2.36	0.54
1:B:72:LEU:CD1	1:B:337:ARG:HD2	2.37	0.54
1:B:208:LEU:HD12	1:B:209:PRO:HD2	1.89	0.54
1:A:117:ALA:O	1:A:121:MET:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASP:O	1:B:163:ARG:HB2	2.08	0.53
1:B:285:GLY:HA2	1:B:290:THR:CG2	2.37	0.53
1:B:75:ARG:H	1:B:75:ARG:NE	2.05	0.53
1:B:325:PHE:CE1	1:B:347:MET:HG2	2.43	0.53
1:A:162:ASP:O	1:A:163:ARG:HB2	2.08	0.53
1:A:46:MET:HE1	1:A:355:PRO:CA	2.39	0.53
1:A:304:LEU:HD22	1:A:308:PHE:HB2	1.90	0.52
1:B:105:HIS:CG	1:B:226:ARG:NH1	2.79	0.51
1:A:80:TYR:O	1:A:82:PRO:HD3	2.10	0.51
1:A:159:LEU:HD13	1:A:161:PHE:CZ	2.47	0.50
1:A:164:HIS:CG	1:A:165:PRO:HD2	2.46	0.50
1:B:87:TYR:OH	1:B:130:MET:HG3	2.12	0.50
1:B:299:ALA:HB1	1:B:300:PRO:CD	2.41	0.50
1:B:72:LEU:HD11	1:B:337:ARG:HD2	1.93	0.49
1:A:140:ALA:HB3	1:A:141:PRO:HD3	1.93	0.49
1:B:105:HIS:ND1	1:B:226:ARG:NH1	2.59	0.49
1:B:130:MET:CB	1:B:131:PRO:HD3	2.37	0.49
1:B:164:HIS:CG	1:B:165:PRO:HD2	2.47	0.49
1:A:285:GLY:HA2	1:A:290:THR:CG2	2.42	0.49
1:A:63:THR:O	1:A:67:GLN:HG3	2.13	0.49
1:A:69:LEU:HD11	1:A:341:LEU:HD13	1.95	0.49
1:A:220:ARG:HD2	2:A:400:SO4:O3	2.13	0.49
1:A:46:MET:HE2	1:A:46:MET:HA	1.95	0.48
1:A:178:LEU:HD21	1:A:291:LEU:HD22	1.96	0.48
1:A:203:ILE:HG23	1:A:324:VAL:HG22	1.94	0.48
1:A:187:VAL:O	1:A:191:VAL:HG23	2.13	0.48
1:B:46:MET:HE1	1:B:355:PRO:HB3	1.96	0.48
1:A:79:VAL:HG12	1:A:80:TYR:N	2.29	0.48
1:A:69:LEU:CD1	1:A:341:LEU:HD13	2.43	0.48
1:B:80:TYR:O	1:B:82:PRO:HD3	2.13	0.47
1:A:221:GLN:HB2	4:A:2041:HOH:O	2.14	0.47
1:A:189:ALA:HB2	4:B:2006:HOH:O	2.13	0.47
1:A:246:VAL:O	1:A:250:GLN:HG3	2.14	0.47
1:B:118:ALA:HB1	4:B:2010:HOH:O	2.15	0.46
1:B:281:ARG:HA	1:B:282:PRO:HD3	1.73	0.46
1:B:373:GLY:O	1:B:374:GLU:HB2	2.15	0.46
1:A:62:LYS:O	1:A:66:THR:HG23	2.15	0.46
1:A:46:MET:HE1	1:A:355:PRO:HB3	1.98	0.46
1:A:317:LYS:HA	1:A:320:ARG:HD2	1.97	0.45
1:A:317:LYS:HA	1:A:320:ARG:CD	2.47	0.45
1:A:373:GLY:O	1:A:374:GLU:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:PRO:HB2	1:B:213:HIS:HE1	1.81	0.45
1:A:208:LEU:HD12	1:A:209:PRO:HD2	1.97	0.45
1:A:193:LEU:HD13	1:B:193:LEU:HD13	1.99	0.45
1:B:146:GLU:HG3	1:B:199:PRO:HB3	1.99	0.44
1:B:203:ILE:HG23	1:B:324:VAL:HG22	1.99	0.44
1:A:61:GLY:HA2	1:A:220:ARG:NH1	2.32	0.44
1:A:327:LEU:HD23	1:A:329:TYR:CZ	2.52	0.44
1:B:66:THR:HG23	1:B:160:ILE:CG2	2.39	0.44
1:A:299:ALA:HB1	1:A:300:PRO:HD2	2.00	0.43
1:A:237:ARG:O	1:A:241:LEU:HG	2.18	0.43
1:B:164:HIS:O	1:B:165:PRO:C	2.62	0.43
1:B:211:ASP:O	1:B:215:ASP:HB2	2.18	0.43
1:A:46:MET:HE1	1:A:355:PRO:CB	2.49	0.43
1:B:46:MET:HA	1:B:46:MET:HE2	2.01	0.43
1:A:49:LEU:HD13	1:A:157:LEU:HD23	2.01	0.42
1:B:79:VAL:HG12	1:B:80:TYR:N	2.34	0.42
1:B:251:CYS:HB2	1:B:281:ARG:HB2	2.01	0.42
1:A:182:MET:HE2	1:A:182:MET:HB2	1.92	0.42
1:B:358:ILE:CB	1:B:359:PRO:HD3	2.42	0.42
1:B:121:MET:HB3	1:B:182:MET:HE2	2.01	0.42
1:B:237:ARG:O	1:B:241:LEU:HG	2.20	0.42
1:B:262:LEU:HD22	1:B:290:THR:CG2	2.50	0.42
1:A:211:ASP:O	1:A:215:ASP:HB2	2.19	0.42
1:B:357:SER:O	1:B:361:ILE:HG13	2.20	0.42
1:A:126:ILE:HD11	1:B:126:ILE:HD11	2.02	0.42
1:A:364:LEU:HD22	1:B:310:TRP:CZ2	2.55	0.42
1:A:262:LEU:HB3	1:A:293:ARG:HD3	2.02	0.41
1:A:198:LEU:HB3	1:A:199:PRO:HD2	2.02	0.41
1:B:74:SER:HB3	1:B:77:ASP:CG	2.45	0.41
1:A:130:MET:CB	1:A:131:PRO:HD3	2.47	0.41
1:B:337:ARG:HH11	1:B:337:ARG:HD3	1.68	0.41
1:A:101:TYR:CZ	1:A:225:GLU:HG3	2.56	0.41
1:A:222:ARG:HB3	1:A:223:PRO:HD2	2.01	0.41
1:B:317:LYS:HA	1:B:320:ARG:HD2	2.03	0.41
1:B:327:LEU:HD23	1:B:329:TYR:CZ	2.56	0.41
1:A:63:THR:HG22	1:A:67:GLN:OE1	2.21	0.41
1:A:198:LEU:HB3	1:A:199:PRO:CD	2.51	0.41
1:B:142:HIS:HA	1:B:353:THR:OG1	2.21	0.41
1:B:235:ILE:HD12	1:B:235:ILE:HA	1.83	0.41
1:B:320:ARG:HG3	1:B:320:ARG:HH11	1.86	0.40
1:A:57:PRO:HB2	1:A:213:HIS:HE1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ALA:HB3	1:B:141:PRO:CD	2.50	0.40
1:A:148:GLY:O	1:A:149:SER:C	2.65	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	298/331 (90%)	282 (95%)	16 (5%)	0	100	100
1	B	306/331 (92%)	287 (94%)	17 (6%)	2 (1%)	18	34
All	All	604/662 (91%)	569 (94%)	33 (6%)	2 (0%)	36	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	ALA
1	B	263	SER

5.3.2 Protein sidechains [i](#)

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	248/264 (94%)	233 (94%)	15 (6%)	17	36
1	B	252/264 (96%)	240 (95%)	12 (5%)	23	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	500/528 (95%)	473 (95%)	27 (5%)	20	41

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	62	LYS
1	A	75	ARG
1	A	121	MET
1	A	130	MET
1	A	160	ILE
1	A	182	MET
1	A	212	ARG
1	A	215	ASP
1	A	219	LYS
1	A	247	ARG
1	A	290	THR
1	A	293	ARG
1	A	304	LEU
1	A	307	VAL
1	B	46	MET
1	B	62	LYS
1	B	69	LEU
1	B	75	ARG
1	B	130	MET
1	B	165	PRO
1	B	212	ARG
1	B	215	ASP
1	B	247	ARG
1	B	290	THR
1	B	293	ARG
1	B	307	VAL

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

Mol	Chain	Res	Type
1	A	67	GLN
1	A	351	HIS
1	B	261	GLN
1	B	275	GLN
1	B	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	THM	B	500	-	18,18,18	1.64	2 (11%)	26,26,26	3.08	11 (42%)
2	SO4	B	400	-	4,4,4	0.74	0	6,6,6	0.14	0
3	THM	A	500	-	18,18,18	1.45	3 (16%)	26,26,26	2.63	10 (38%)
2	SO4	A	400	-	4,4,4	0.69	0	6,6,6	0.15	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	THM	B	500	-	-	2/6/18/18	0/2/2/2
3	THM	A	500	-	-	2/6/18/18	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	500	THM	C4-C5	-4.22	1.38	1.44
3	B	500	THM	C2-N1	-3.38	1.33	1.38
3	A	500	THM	C4-C5	-3.32	1.39	1.44
3	A	500	THM	O4'-C1'	2.06	1.47	1.42
3	A	500	THM	C2-N3	2.06	1.41	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	THM	C6-C5-C4	9.43	125.80	118.02
3	A	500	THM	C6-C5-C4	6.34	123.24	118.02
3	B	500	THM	O4'-C1'-C2'	-5.26	96.42	106.25
3	A	500	THM	O4'-C1'-C2'	-4.90	97.10	106.25
3	A	500	THM	C5M-C5-C6	-4.63	116.59	122.85
3	B	500	THM	C5M-C5-C6	-4.56	116.67	122.85
3	A	500	THM	O4'-C4'-C3'	-4.14	96.22	105.65
3	A	500	THM	C4'-O4'-C1'	4.07	119.18	109.51
3	B	500	THM	C4'-O4'-C1'	4.03	119.07	109.51
3	B	500	THM	C5-C6-N1	-3.82	119.17	123.31
3	B	500	THM	N3-C2-N1	3.75	119.78	114.89
3	B	500	THM	C5-C4-N3	-3.65	112.15	115.32
3	B	500	THM	C2'-C1'-N1	3.37	122.24	113.81
3	A	500	THM	C5-C4-N3	-3.27	112.48	115.32
3	B	500	THM	C4-N3-C2	-3.19	123.15	127.34
3	B	500	THM	O4'-C4'-C3'	-3.13	98.50	105.65
3	A	500	THM	C2'-C1'-N1	2.99	121.30	113.81
3	A	500	THM	O4'-C1'-N1	2.80	112.83	107.86
3	A	500	THM	O4'-C4'-C5'	2.37	114.24	109.22
3	B	500	THM	O4'-C4'-C5'	2.05	113.55	109.22
3	A	500	THM	O4-C4-C5	2.00	127.21	124.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	500	THM	O4'-C4'-C5'-O5'
3	A	500	THM	C3'-C4'-C5'-O5'
3	B	500	THM	O4'-C4'-C5'-O5'
3	B	500	THM	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	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	306/331 (92%)	0.36	14 (4%) 37 33	7, 24, 48, 88	0
1	B	314/331 (94%)	0.52	24 (7%) 20 17	7, 25, 58, 104	0
All	All	620/662 (93%)	0.44	38 (6%) 27 23	7, 24, 56, 104	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	GLY	4.7
1	B	148	GLY	4.3
1	A	148	GLY	4.2
1	B	266	ALA	4.2
1	B	265	THR	4.0
1	A	263	SER	3.9
1	B	263	SER	3.5
1	A	76	ASP	3.5
1	A	264	GLY	3.4
1	A	320	ARG	3.3
1	B	264	GLY	3.3
1	B	267	VAL	3.3
1	B	227	LEU	3.1
1	A	373	GLY	3.1
1	A	374	GLU	3.1
1	B	374	GLU	3.0
1	B	216	ARG	3.0
1	B	217	LEU	3.0
1	B	75	ARG	3.0
1	A	342	GLN	3.0
1	B	247	ARG	2.9
1	B	226	ARG	2.8
1	A	149	SER	2.6
1	B	339	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	76	ASP	2.6
1	B	211	ASP	2.5
1	B	320	ARG	2.5
1	B	277	ASN	2.3
1	A	75	ARG	2.3
1	A	46	MET	2.2
1	B	154	PRO	2.2
1	A	356	GLY	2.2
1	A	153	PRO	2.1
1	B	301	ASN	2.1
1	A	65	THR	2.1
1	B	153	PRO	2.1
1	B	149	SER	2.0
1	B	281	ARG	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	THM	A	500	17/17	0.86	0.12	31,33,37,37	0
3	THM	B	500	17/17	0.87	0.12	44,46,49,51	0
2	SO4	A	400	5/5	0.95	0.07	30,30,34,35	0
2	SO4	B	400	5/5	0.95	0.08	26,27,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.