



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:54 PM UTC

PDB ID : 1E2H / pdb_00001e2h
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 : 1.90 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

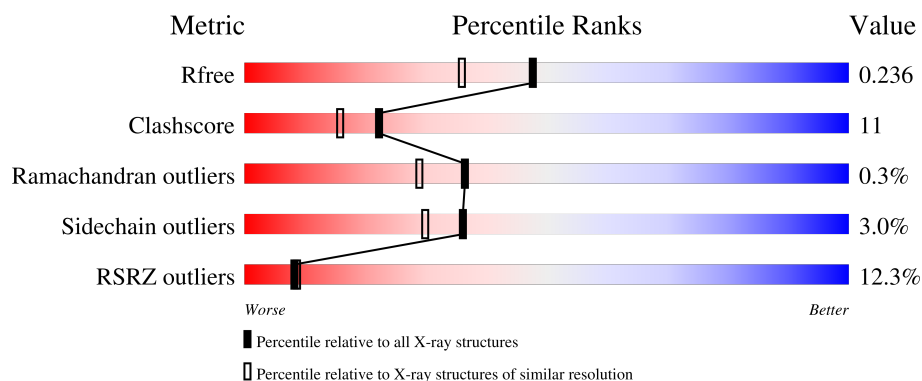
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	8% 73% 17% • 8%
1	B	331	15% 67% 23% • • 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4998 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
			2347	1495	411	425	16			
1	B	311	Total	C	N	O	S	0	0	0
			2365	1507	411	431	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	B	1	Total	O	S	0	0
			5	4	1		

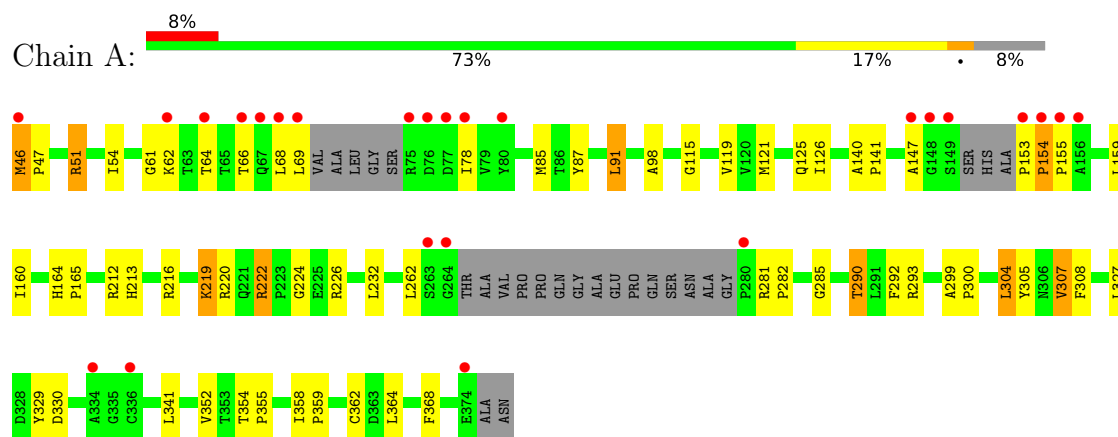
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	143	Total 143	O 143	0	0
3	B	133	Total 133	O 133	0	0

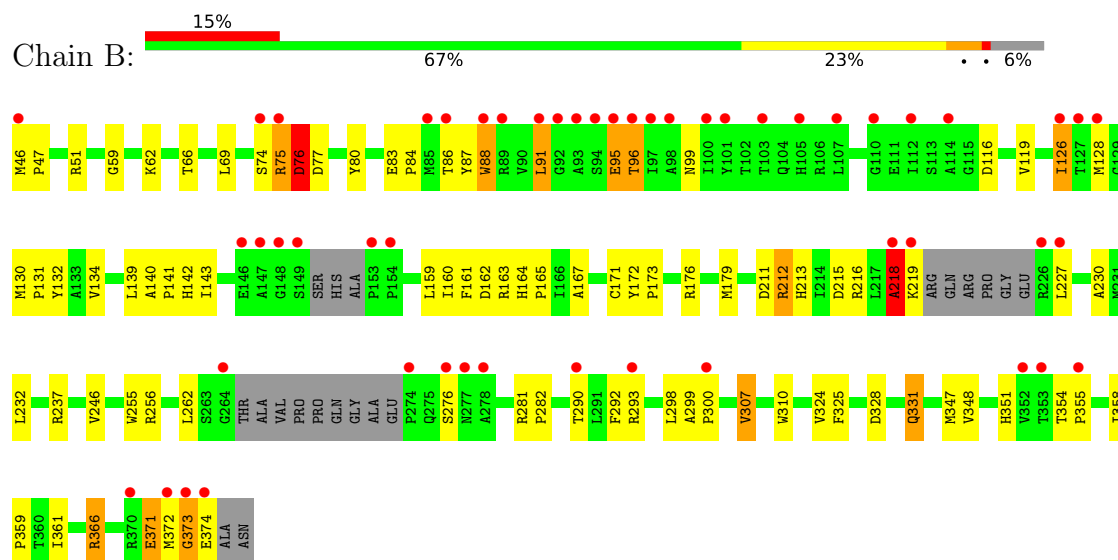
3 Residue-property plots [i](#)

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	113.90Å 117.30Å 107.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-1.90) 99.2 (20.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.47 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.249 0.209 , 0.236	Depositor DCC
R_{free} test set	2873 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4998	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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	0.59	1/2401 (0.0%)	1.31	15/3273 (0.5%)
1	B	0.73	2/2419 (0.1%)	1.42	25/3300 (0.8%)
All	All	0.67	3/4820 (0.1%)	1.37	40/6573 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	THR	N-CA	21.21	1.73	1.46
1	A	154	PRO	CA-C	-8.00	1.44	1.52
1	B	99	ASN	CG-OD1	5.20	1.33	1.23

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	GLN	OE1-CD-NE2	-25.72	96.88	122.60
1	A	153	PRO	CA-C-N	-17.76	102.09	120.38
1	A	153	PRO	C-N-CA	-17.76	102.09	120.38
1	B	95	GLU	CA-C-N	-15.53	96.70	120.31
1	B	95	GLU	C-N-CA	-15.53	96.70	120.31
1	A	154	PRO	N-CA-C	13.79	127.52	110.70
1	B	331	GLN	CG-CD-OE1	12.01	144.83	120.80
1	B	91	LEU	N-CA-C	9.71	121.46	111.07
1	B	307	VAL	CB-CA-C	-9.30	99.98	111.88
1	A	307	VAL	CB-CA-C	-9.15	100.25	111.97
1	B	88	TRP	N-CA-C	8.16	120.26	111.36
1	A	51	ARG	CD-NE-CZ	8.12	135.76	124.40
1	B	237	ARG	CD-NE-CZ	7.85	135.40	124.40
1	A	292	PHE	CA-CB-CG	-7.76	106.04	113.80
1	B	331	GLN	CB-CG-CD	7.69	125.68	112.60
1	B	218	ALA	CA-C-N	7.55	135.29	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ALA	C-N-CA	7.55	135.29	121.70
1	B	96	THR	N-CA-CB	-7.22	99.09	110.28
1	A	91	LEU	N-CA-C	6.65	118.19	111.07
1	B	51	ARG	CD-NE-CZ	6.55	133.57	124.40
1	B	76	ASP	CA-CB-CG	6.54	119.14	112.60
1	A	290	THR	N-CA-CB	6.53	120.28	110.22
1	A	368	PHE	CA-CB-CG	6.08	119.89	113.80
1	A	290	THR	CB-CA-C	-6.02	99.50	110.63
1	A	293	ARG	N-CA-C	-5.97	102.38	110.68
1	A	226	ARG	CD-NE-CZ	5.91	132.68	124.40
1	A	147	ALA	N-CA-C	-5.88	106.27	113.50
1	B	171	CYS	N-CA-C	5.79	117.27	111.07
1	B	161	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	222	ARG	CD-NE-CZ	5.76	132.46	124.40
1	B	307	VAL	N-CA-CB	5.72	116.86	110.51
1	B	292	PHE	CA-CB-CG	-5.63	108.17	113.80
1	B	351	HIS	N-CA-C	-5.52	103.41	110.53
1	B	88	TRP	CA-CB-CG	5.42	123.90	113.60
1	B	371	GLU	N-CA-C	5.42	118.35	111.69
1	B	348	VAL	N-CA-C	5.36	115.96	108.89
1	B	116	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	143	ILE	N-CA-C	5.10	115.44	107.99
1	A	352	VAL	CA-C-O	-5.09	117.66	121.68
1	B	134	VAL	N-CA-CB	5.01	118.09	110.58

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	2347	0	2364	42	0
1	B	2365	0	2381	62	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	143	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	133	0	0	3	0
All	All	4998	0	4745	100	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 11.

All (100) 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:B:96:THR:CA	1:B:96:THR:N	1.73	1.51
1:B:95:GLU:C	1:B:96:THR:CA	2.31	1.03
1:B:354:THR:HB	1:B:355:PRO:HD2	1.49	0.94
1:A:358:ILE:HB	1:A:359:PRO:HD3	1.65	0.79
1:B:212:ARG:HH21	1:B:215:ASP:HB3	1.47	0.78
1:B:276:SER:HB2	1:B:324:VAL:HB	1.64	0.77
1:B:96:THR:N	1:B:96:THR:CB	2.49	0.75
1:A:354:THR:HB	1:A:355:PRO:HD2	1.69	0.75
1:B:328:ASP:O	1:B:331:GLN:NE2	2.20	0.75
1:B:373:GLY:O	1:B:374:GLU:HB2	1.86	0.73
1:B:95:GLU:O	1:B:96:THR:CA	2.36	0.72
1:B:75:ARG:HD2	1:B:75:ARG:H	1.55	0.71
1:A:262:LEU:HD22	1:A:290:THR:HG22	1.72	0.70
1:A:285:GLY:HA2	1:A:290:THR:HG23	1.74	0.70
1:A:46:MET:HE2	1:A:46:MET:HA	1.75	0.68
1:A:212:ARG:NH2	1:A:216:ARG:HH21	1.92	0.67
1:A:285:GLY:HA2	1:A:290:THR:CG2	2.25	0.66
1:A:119:VAL:HG12	1:B:119:VAL:HG12	1.77	0.66
1:A:61:GLY:HA2	1:A:220:ARG:NH1	2.11	0.66
1:B:46:MET:N	1:B:47:PRO:HD3	2.10	0.65
1:B:86:THR:HB	1:B:372:MET:HA	1.79	0.64
1:B:354:THR:HB	1:B:355:PRO:CD	2.25	0.64
1:A:290:THR:HG21	3:A:2108:HOH:O	1.98	0.63
1:B:86:THR:O	1:B:91:LEU:HG	1.99	0.62
1:B:262:LEU:HD22	1:B:290:THR:HG23	1.82	0.61
1:B:46:MET:N	1:B:47:PRO:CD	2.64	0.60
1:B:88:TRP:HZ2	1:B:132:TYR:HH	1.50	0.57
1:B:139:LEU:HD11	1:B:361:ILE:HG23	1.87	0.57
1:B:212:ARG:NH2	1:B:215:ASP:HB3	2.18	0.56
1:A:164:HIS:CG	1:A:165:PRO:HD2	2.41	0.55
1:B:84:PRO:HA	1:B:372:MET:O	2.06	0.55
1:B:159:LEU:HD11	1:B:361:ILE:CG2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HG13	1:A:66:THR:HG21	1.88	0.55
1:A:61:GLY:HA2	1:A:220:ARG:HH11	1.71	0.55
1:A:126:ILE:HD11	1:B:126:ILE:HG13	1.89	0.54
1:A:69:LEU:HD11	1:A:341:LEU:HD13	1.88	0.54
1:B:66:THR:HG21	1:B:80:TYR:CE1	2.42	0.54
1:B:95:GLU:O	1:B:96:THR:C	2.50	0.54
1:A:62:LYS:NZ	1:A:62:LYS:HB2	2.21	0.54
1:A:121:MET:O	1:A:125:GLN:HG2	2.09	0.53
1:B:164:HIS:CG	1:B:165:PRO:HD2	2.44	0.52
1:B:87:TYR:HA	1:B:91:LEU:HB2	1.91	0.52
1:A:281:ARG:HB2	1:A:282:PRO:HD2	1.92	0.52
1:B:246:VAL:HG21	1:B:324:VAL:HG21	1.92	0.52
1:A:54:ILE:HG13	1:A:66:THR:CG2	2.40	0.51
1:B:142:HIS:HB3	1:B:361:ILE:HD11	1.92	0.51
1:B:88:TRP:HZ2	1:B:132:TYR:OH	1.93	0.51
1:A:213:HIS:CE1	1:A:232:LEU:HD11	2.47	0.50
1:A:364:LEU:HD22	1:B:310:TRP:CZ2	2.47	0.49
1:B:66:THR:HG23	1:B:160:ILE:HG21	1.94	0.49
1:A:87:TYR:HA	1:A:91:LEU:HB2	1.95	0.48
1:A:85:MET:HE1	1:A:222:ARG:HD3	1.95	0.48
1:A:212:ARG:HD3	1:A:330:ASP:OD1	2.13	0.47
1:B:211:ASP:OD1	1:B:212:ARG:N	2.47	0.47
1:B:366:ARG:HD2	3:B:2129:HOH:O	2.14	0.47
1:A:304:LEU:HD22	1:A:308:PHE:HB2	1.96	0.47
1:A:64:THR:O	1:A:68:LEU:HG	2.14	0.47
1:B:140:ALA:HB3	1:B:141:PRO:HD3	1.97	0.47
1:B:167:ALA:HB3	3:B:2046:HOH:O	2.14	0.46
1:B:371:GLU:HG2	1:B:372:MET:HG3	1.98	0.46
1:B:83:GLU:HB2	1:B:162:ASP:OD2	2.16	0.46
1:B:96:THR:N	1:B:96:THR:C	2.65	0.46
1:B:281:ARG:HA	1:B:282:PRO:HD3	1.82	0.46
1:B:86:THR:CB	1:B:372:MET:HA	2.45	0.45
1:B:86:THR:HG22	1:B:91:LEU:HG	1.98	0.45
1:A:78:ILE:HD11	1:A:160:ILE:HD12	1.97	0.45
1:A:212:ARG:HH22	1:A:216:ARG:HH21	1.62	0.45
1:A:305:TYR:CE2	1:B:91:LEU:HD22	2.52	0.45
1:A:69:LEU:CD1	1:A:341:LEU:HD13	2.48	0.44
1:B:59:GLY:O	1:B:216:ARG:HD3	2.18	0.44
1:B:262:LEU:HB3	1:B:293:ARG:HD3	1.99	0.44
1:A:51:ARG:HG3	3:A:2001:HOH:O	2.18	0.44
1:B:96:THR:HG21	1:B:128:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:THR:O	1:B:293:ARG:HG3	2.18	0.44
1:B:325:PHE:CE2	1:B:347:MET:HG2	2.53	0.44
1:B:69:LEU:C	1:B:69:LEU:HD13	2.43	0.43
1:A:46:MET:HA	1:A:47:PRO:HD3	1.86	0.43
1:B:172:TYR:N	1:B:173:PRO:CD	2.81	0.43
1:B:373:GLY:O	1:B:374:GLU:CB	2.59	0.43
1:B:130:MET:HB3	1:B:131:PRO:HD3	2.01	0.43
1:B:76:ASP:HB3	3:B:2013:HOH:O	2.18	0.43
1:A:219:LYS:NZ	1:A:219:LYS:HB3	2.34	0.42
1:A:98:ALA:HB2	1:A:224:GLY:HA3	2.00	0.42
1:B:299:ALA:HB1	1:B:300:PRO:CD	2.49	0.42
1:A:327:LEU:HD23	1:A:329:TYR:CZ	2.54	0.42
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.96	0.42
1:A:140:ALA:HB3	1:A:141:PRO:HD3	2.02	0.42
1:A:299:ALA:HB1	1:A:300:PRO:CD	2.49	0.41
1:A:62:LYS:HB2	1:A:62:LYS:HZ2	1.85	0.41
1:B:162:ASP:O	1:B:163:ARG:HB2	2.20	0.41
1:A:364:LEU:C	1:A:364:LEU:HD13	2.44	0.41
1:B:74:SER:HB3	1:B:77:ASP:CG	2.46	0.41
1:B:179:MET:HE1	1:B:230:ALA:HB3	2.01	0.41
1:A:299:ALA:HB1	1:A:300:PRO:HD2	2.03	0.41
1:B:358:ILE:N	1:B:359:PRO:HD2	2.35	0.41
1:B:218:ALA:O	1:B:219:LYS:HG3	2.21	0.40
1:A:115:GLY:O	1:A:119:VAL:HG23	2.21	0.40
1:B:176:ARG:HD3	1:B:176:ARG:HA	1.96	0.40
1:B:213:HIS:CE1	1:B:232:LEU:HD11	2.57	0.40
1:B:255:TRP:CE2	1:B:256:ARG:HG3	2.57	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	298/331 (90%)	290 (97%)	8 (3%)	0	100	100
1	B	303/331 (92%)	291 (96%)	10 (3%)	2 (1%)	18	10
All	All	601/662 (91%)	581 (97%)	18 (3%)	2 (0%)	36	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	ALA
1	B	373	GLY

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	248/264 (94%)	242 (98%)	6 (2%)	43	38
1	B	250/264 (95%)	241 (96%)	9 (4%)	31	23
All	All	498/528 (94%)	483 (97%)	15 (3%)	36	30

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	159	LEU
1	A	219	LYS
1	A	304	LEU
1	A	307	VAL
1	A	362	CYS
1	B	62	LYS
1	B	75	ARG
1	B	76	ASP
1	B	126	ILE
1	B	212	ARG
1	B	227	LEU
1	B	298	LEU
1	B	307	VAL

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Mol	Chain	Res	Type
1	B	366	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	HIS
1	B	67	GLN
1	B	99	ASN
1	B	349	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](#)

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	400	-	4,4,4	0.71	0	6,6,6	0.19	0
2	SO4	B	400	-	4,4,4	0.82	0	6,6,6	0.33	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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	25 (8%) 17 18	15, 27, 58, 116	0
1	B	311/331 (93%)	0.69	51 (16%) 4 4	14, 28, 69, 106	0
All	All	617/662 (93%)	0.53	76 (12%) 8 9	14, 27, 66, 116	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	GLY	10.2
1	B	372	MET	6.7
1	A	148	GLY	6.2
1	A	69	LEU	5.5
1	B	374	GLU	5.2
1	A	149	SER	4.8
1	B	96	THR	4.8
1	A	153	PRO	4.8
1	B	153	PRO	4.5
1	B	91	LEU	4.5
1	B	276	SER	4.5
1	A	68	LEU	4.3
1	A	264	GLY	4.3
1	B	112	ILE	4.0
1	B	92	GLY	3.9
1	B	107	LEU	3.8
1	B	227	LEU	3.8
1	B	85	MET	3.8
1	B	277	ASN	3.7
1	B	219	LYS	3.7
1	B	226	ARG	3.7
1	B	147	ALA	3.6
1	B	148	GLY	3.6
1	A	75	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	110	GLY	3.5
1	A	280	PRO	3.5
1	A	66	THR	3.5
1	A	147	ALA	3.5
1	B	100	ILE	3.5
1	A	154	PRO	3.4
1	A	80	TYR	3.4
1	B	97	ILE	3.3
1	B	46	MET	3.3
1	B	274	PRO	3.3
1	B	218	ALA	3.2
1	A	76	ASP	3.2
1	B	127	THR	3.2
1	B	101	TYR	3.2
1	A	374	GLU	2.9
1	A	62	LYS	2.9
1	B	89	ARG	2.9
1	B	93	ALA	2.9
1	B	86	THR	2.8
1	B	353	THR	2.8
1	B	370	ARG	2.8
1	B	355	PRO	2.8
1	A	46	MET	2.8
1	B	98	ALA	2.7
1	B	264	GLY	2.7
1	A	263	SER	2.6
1	B	75	ARG	2.6
1	B	146	GLU	2.5
1	A	78	ILE	2.5
1	A	334	ALA	2.5
1	B	149	SER	2.5
1	B	278	ALA	2.5
1	B	352	VAL	2.4
1	B	293	ARG	2.4
1	B	88	TRP	2.4
1	A	67	GLN	2.4
1	A	77	ASP	2.3
1	A	156	ALA	2.3
1	B	94	SER	2.2
1	B	290	THR	2.2
1	A	336	CYS	2.2
1	B	114	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	95	GLU	2.1
1	A	64	THR	2.1
1	B	105	HIS	2.1
1	B	154	PRO	2.1
1	B	300	PRO	2.1
1	B	126	ILE	2.0
1	B	103	THR	2.0
1	B	74	SER	2.0
1	B	128	MET	2.0
1	A	155	PRO	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(Å ²)	Q<0.9
2	SO4	A	400	5/5	0.94	0.10	40,43,45,47	0
2	SO4	B	400	5/5	0.96	0.08	28,30,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.