Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:29 PM GMT

PDB ID : 1KI4
Title : CRYSTAL STRUCTURE OF THYMIDINE KINASE FROM HERPES SIM-
PLEX VIRUS TYPE I COMPLEXED WITH 5-BROMOTHIENYLDEOXY
URIDINE
Authors : Champness, J.N.; Bennett, M.S.; Wien, F.; Visse, R.; Summers, W.C.; Sander-
son, M.R.
Deposited on : 1998-05-18
Resolution : 2.34 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		24
Ramachandran outliers		0.2%
Sidechain outliers		9.3%
RSRZ outliers		0.7%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
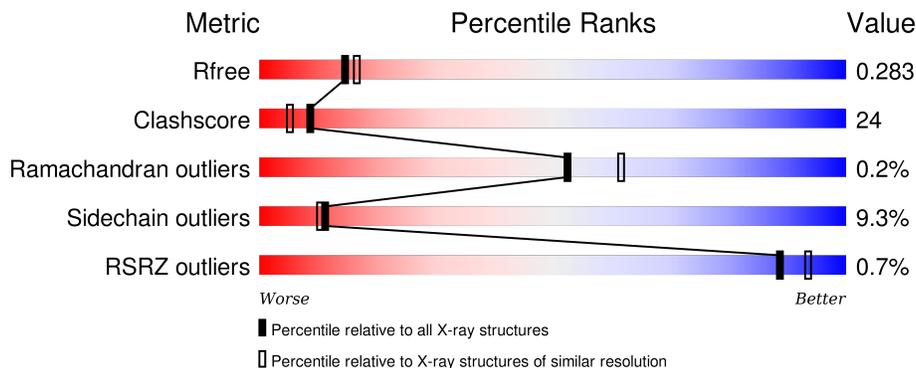
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	52% 34% 5% 8%
1	B	331	% 53% 35% 5% 7%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 4942 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	303	Total 2303	C 1467	N 405	O 416	S 15	0	0	3
1	B	307	Total 2322	C 1482	N 406	O 419	S 15	0	0	3

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
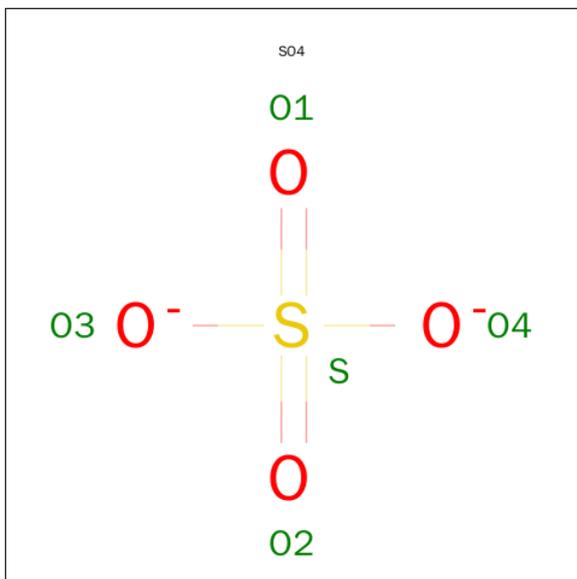
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is 5-BROMOTHIENYLDEOXYURIDINE (three-letter code: BTD) (formula: $C_{13}H_{13}BrN_2O_5S$).
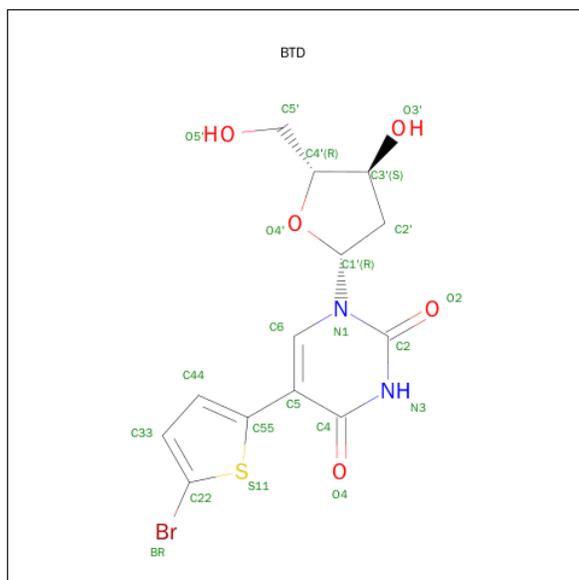
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	S	0	0
			22	1	13	2	5	1		
3	B	1	Total	Br	C	N	O	S	0	0
			22	1	13	2	5	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	132	Total	O	0	0
			132	132		
4	B	131	Total	O	0	0
			131	131		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
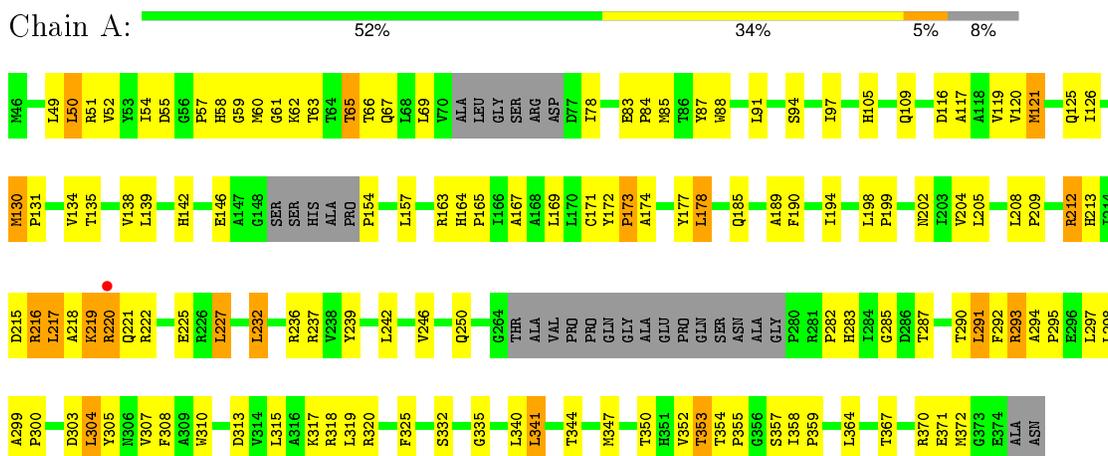
- Molecule 1: THYMIDINE KINASE
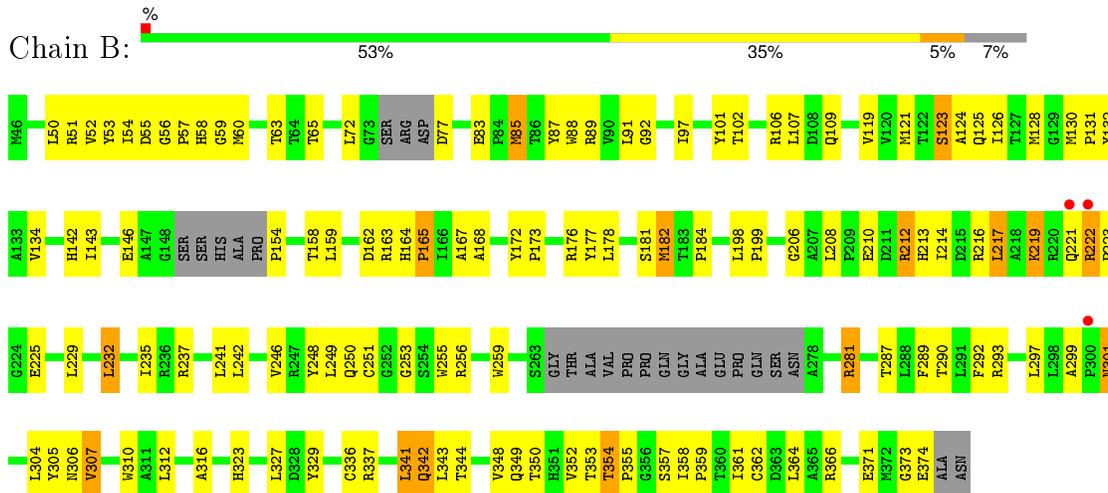
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	114.10Å 116.00Å 108.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.34 14.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	83.0 (12.00-2.34) 79.4 (14.98-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.24Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.210 , 0.309 0.200 , 0.283	Depositor DCC
R_{free} test set	2516 reflections (11.02%)	DCC
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 77.3	EDS
Estimated twinning fraction	0.057 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 27398 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4942	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BTD, 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	0.69	0/2354	0.84	3/3213 (0.1%)
1	B	0.72	0/2374	0.85	1/3243 (0.0%)
All	All	0.70	0/4728	0.84	4/6456 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	PRO	N-CA-CB	5.46	109.85	103.30
1	A	293	ARG	N-CA-C	-5.45	96.29	111.00
1	B	154	PRO	N-CA-CB	5.45	109.84	103.30
1	A	291	LEU	CA-CB-CG	5.06	126.93	115.30

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	2303	0	2310	120	0
1	B	2322	0	2332	108	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	22	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	22	0	12	5	0
4	A	132	0	0	14	1
4	B	131	0	0	11	1
All	All	4942	0	4667	221	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 24.

All (221) 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:69:LEU:HD11	1:A:340:LEU:HG	1.53	0.91
1:B:65:THR:HG21	1:B:336:CYS:HB2	1.54	0.87
1:B:59:GLY:HA3	1:B:217:LEU:HD22	1.56	0.86
1:B:208:LEU:HD11	1:B:212:ARG:HD2	1.60	0.82
1:A:87:TYR:HA	1:A:91:LEU:HB2	1.62	0.82
1:B:214:ILE:HG13	1:B:229:LEU:HD22	1.61	0.81
1:B:58:HIS:HB3	4:B:693:HOH:O	1.77	0.81
1:A:216:ARG:O	1:A:219:LYS:HD3	1.83	0.78
1:A:55:ASP:O	1:A:205:LEU:HA	1.84	0.78
1:B:159:LEU:HD11	1:B:361:ILE:CG2	2.15	0.76
1:A:117:ALA:O	1:A:121:MET:HB2	1.85	0.75
1:B:143:ILE:HG13	1:B:198:LEU:HD13	1.67	0.75
1:A:246:VAL:O	1:A:250:GLN:HG3	1.87	0.74
1:A:49:LEU:HD12	1:A:157:LEU:O	1.88	0.73
1:B:287:THR:O	1:B:290:THR:HG22	1.90	0.71
1:A:213:HIS:CE1	1:A:232:LEU:HD21	2.27	0.69
1:B:142:HIS:HA	1:B:353:THR:HB	1.74	0.69
1:A:97:ILE:HG13	4:A:539:HOH:O	1.92	0.68
1:A:217:LEU:HD13	1:A:227:LEU:HD23	1.75	0.68
1:B:249:LEU:HD21	1:B:316:ALA:HB1	1.74	0.68
1:A:353:THR:HG22	1:A:354:THR:HG23	1.77	0.67
1:B:354:THR:HG22	1:B:355:PRO:HD2	1.78	0.66
1:A:119:VAL:HG23	1:B:123:SER:HB2	1.78	0.65
1:B:85:MET:HE3	1:B:88:TRP:HE3	1.61	0.65
1:A:119:VAL:HG23	1:B:123:SER:CB	2.27	0.65
1:A:217:LEU:HD12	1:A:232:LEU:HG	1.79	0.65
1:A:208:LEU:HD12	1:A:209:PRO:HD2	1.78	0.65
1:B:59:GLY:HA3	1:B:217:LEU:CD2	2.26	0.64
1:B:357:SER:O	1:B:361:ILE:HG13	1.97	0.64
1:A:287:THR:O	1:A:290:THR:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HH21	1:A:172:TYR:HE1	1.43	0.64
1:A:58:HIS:CD2	1:A:58:HIS:H	2.14	0.64
1:A:205:LEU:HD22	1:A:239:TYR:HD1	1.62	0.64
1:A:126:ILE:HD11	1:B:126:ILE:HD11	1.81	0.62
1:B:242:LEU:O	1:B:246:VAL:HG23	1.99	0.62
1:A:364:LEU:HD12	1:B:310:TRP:CZ2	2.34	0.62
1:B:165:PRO:HD3	4:B:547:HOH:O	2.00	0.62
1:B:214:ILE:HD12	1:B:232:LEU:HD13	1.80	0.61
1:B:222:ARG:HG3	1:B:223:PRO:HD2	1.81	0.61
3:B:2:BTD:O5'	3:B:2:BTD:H6	2.01	0.61
1:A:222:ARG:O	1:A:225:GLU:HG3	2.01	0.60
1:B:58:HIS:HD2	1:B:172:TYR:OH	1.84	0.60
1:B:348:VAL:HG23	4:B:640:HOH:O	2.00	0.60
1:A:213:HIS:NE2	1:A:232:LEU:HD21	2.17	0.60
1:A:163:ARG:NH1	4:A:570:HOH:O	2.33	0.60
1:A:164:HIS:CG	1:A:165:PRO:HD2	2.37	0.60
4:A:581:HOH:O	1:B:119:VAL:HG22	2.02	0.60
1:B:219:LYS:HA	1:B:219:LYS:HE3	1.84	0.59
1:B:168:ALA:HB2	3:B:2:BTD:S11	2.43	0.59
1:B:237:ARG:O	1:B:241:LEU:HG	2.02	0.59
1:B:358:ILE:HB	1:B:359:PRO:HD3	1.84	0.59
1:A:205:LEU:HD22	1:A:239:TYR:CD1	2.38	0.59
3:A:1:BTD:S11	3:A:1:BTD:O4	2.61	0.59
1:B:362:CYS:O	1:B:366:ARG:HG3	2.03	0.59
1:B:56:GLY:O	1:B:163:ARG:NH2	2.37	0.58
1:A:130:MET:O	1:A:134:VAL:HG22	2.03	0.58
1:A:315:LEU:HD11	1:A:319:LEU:HD11	1.86	0.58
1:A:232:LEU:O	1:A:236:ARG:HG3	2.03	0.58
1:B:342:GLN:HG3	1:B:343:LEU:N	2.18	0.57
1:B:51:ARG:NH2	1:B:199:PRO:O	2.38	0.57
1:B:132:TYR:OH	3:B:2:BTD:H33	2.04	0.57
1:A:364:LEU:HD12	1:B:310:TRP:CE2	2.40	0.57
1:B:130:MET:O	1:B:134:VAL:HG13	2.05	0.56
1:A:51:ARG:NH2	1:A:199:PRO:O	2.38	0.56
1:B:159:LEU:HD11	1:B:361:ILE:HG21	1.86	0.56
1:A:119:VAL:HG22	1:B:119:VAL:HG12	1.87	0.56
1:A:358:ILE:HB	1:A:359:PRO:HD3	1.87	0.56
1:A:83:GLU:HG2	1:A:88:TRP:HH2	1.71	0.56
1:A:63:THR:O	1:A:67:GLN:HG3	2.05	0.56
1:B:89:ARG:HG2	4:B:540:HOH:O	2.05	0.56
1:B:163:ARG:NH1	4:B:693:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HD13	1:A:227:LEU:CD2	2.35	0.56
1:B:177:TYR:CE1	1:B:184:PRO:HD3	2.41	0.55
1:B:102:THR:O	1:B:106:ARG:HG2	2.07	0.55
1:B:87:TYR:HA	1:B:91:LEU:HB2	1.88	0.55
1:A:125:GLN:HG3	1:A:173:PRO:HG3	1.89	0.55
1:B:221:GLN:HB2	4:B:683:HOH:O	2.06	0.55
1:A:59:GLY:O	1:A:216:ARG:HB3	2.07	0.54
1:A:66:THR:HG22	1:A:340:LEU:HD21	1.89	0.54
1:B:159:LEU:HD11	1:B:361:ILE:HG22	1.88	0.54
1:A:142:HIS:HE1	4:A:625:HOH:O	1.90	0.54
1:A:54:ILE:HG12	1:A:66:THR:CG2	2.38	0.54
1:B:289:PHE:HD1	1:B:312:LEU:HD22	1.73	0.54
1:B:60:MET:SD	1:B:206:GLY:O	2.66	0.53
1:B:292:PHE:CD2	1:B:312:LEU:HD21	2.43	0.53
1:B:216:ARG:O	1:B:219:LYS:HB3	2.08	0.53
1:B:50:LEU:HD13	1:B:52:VAL:HG23	1.90	0.53
1:B:130:MET:HB3	1:B:131:PRO:HD3	1.90	0.53
1:A:212:ARG:NH1	1:A:216:ARG:NH2	2.56	0.53
1:A:83:GLU:HG2	1:A:88:TRP:CH2	2.43	0.53
1:B:299:ALA:HA	1:B:305:TYR:CZ	2.44	0.53
1:B:72:LEU:HD21	1:B:337:ARG:HD3	1.90	0.52
1:A:305:TYR:HB2	1:A:308:PHE:CD2	2.44	0.52
1:B:142:HIS:O	1:B:353:THR:N	2.43	0.52
1:A:209:PRO:HD3	4:A:613:HOH:O	2.09	0.52
1:B:77:ASP:N	4:B:674:HOH:O	2.42	0.51
1:A:367:THR:HG23	1:A:370:ARG:HH21	1.75	0.51
1:B:352:VAL:HB	1:B:357:SER:HB2	1.92	0.51
1:B:222:ARG:H	1:B:225:GLU:HB3	1.75	0.51
1:B:72:LEU:CD2	1:B:337:ARG:HD3	2.40	0.51
1:A:57:PRO:HD2	1:A:60:MET:CE	2.41	0.51
1:B:132:TYR:CZ	3:B:2:BTD:H33	2.45	0.51
1:A:66:THR:O	1:A:69:LEU:HB2	2.11	0.51
1:A:85:MET:HE1	1:A:97:ILE:HD12	1.92	0.51
1:A:282:PRO:HA	4:A:556:HOH:O	2.10	0.51
1:B:65:THR:HG21	1:B:336:CYS:CB	2.36	0.50
1:A:164:HIS:CD2	1:A:165:PRO:HD2	2.47	0.50
1:B:256:ARG:HD2	4:B:603:HOH:O	2.11	0.50
1:A:54:ILE:N	1:A:54:ILE:HD12	2.25	0.50
1:A:87:TYR:HB2	1:A:372:MET:HG2	1.93	0.50
1:A:298:LEU:HA	1:A:303:ASP:O	2.11	0.50
1:A:50:LEU:HD13	1:A:52:VAL:HG23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLY:O	1:B:374:GLU:HB2	2.12	0.49
1:B:249:LEU:HD11	1:B:316:ALA:HA	1.94	0.49
1:A:169:LEU:HD23	1:A:190:PHE:CD1	2.47	0.49
1:B:246:VAL:O	1:B:250:GLN:HG3	2.12	0.49
1:B:292:PHE:HD2	1:B:312:LEU:HD21	1.78	0.49
1:A:208:LEU:HD11	1:A:212:ARG:HD2	1.93	0.48
1:A:220:ARG:HA	4:A:714:HOH:O	2.12	0.48
1:A:354:THR:HB	1:A:355:PRO:CD	2.43	0.48
1:A:105:HIS:O	1:A:109:GLN:HG2	2.13	0.48
1:A:178:LEU:HD21	1:A:237:ARG:HD3	1.95	0.48
1:A:185:GLN:HG2	1:B:92:GLY:HA2	1.94	0.48
1:B:289:PHE:CD1	1:B:312:LEU:HD22	2.48	0.48
1:A:216:ARG:O	1:A:217:LEU:C	2.52	0.48
1:A:310:TRP:HA	1:A:313:ASP:OD2	2.13	0.48
1:B:251:CYS:HB2	1:B:281:ARG:HB2	1.96	0.47
1:B:50:LEU:HD23	1:B:349:GLN:HG2	1.95	0.47
1:A:304:LEU:HD22	1:A:308:PHE:HB2	1.96	0.47
1:B:176:ARG:HA	1:B:176:ARG:HD3	1.62	0.47
1:B:337:ARG:O	1:B:341:LEU:HB2	2.14	0.47
1:A:202:ASN:CG	1:A:347:MET:HB3	2.35	0.47
1:B:143:ILE:CG1	1:B:198:LEU:HD13	2.42	0.47
1:A:146:GLU:HA	1:A:350:THR:HG22	1.96	0.47
1:A:222:ARG:NH1	4:A:712:HOH:O	2.47	0.47
1:A:320:ARG:HG2	1:A:320:ARG:O	2.14	0.47
1:A:54:ILE:HG12	1:A:66:THR:HG21	1.96	0.47
1:A:146:GLU:HG3	1:A:199:PRO:HB3	1.97	0.47
1:B:83:GLU:HG3	1:B:162:ASP:OD1	2.15	0.47
1:B:232:LEU:O	1:B:235:ILE:HG22	2.14	0.47
1:B:50:LEU:HD12	1:B:158:THR:HG23	1.96	0.46
1:B:256:ARG:HG2	1:B:256:ARG:HH11	1.80	0.46
1:B:371:GLU:HB2	4:B:656:HOH:O	2.14	0.46
1:B:163:ARG:NH1	4:B:569:HOH:O	2.48	0.46
3:A:1:BTD:H2'1	3:A:1:BTD:O5'	2.16	0.46
1:B:255:TRP:O	1:B:259:TRP:N	2.48	0.46
1:A:292:PHE:C	1:A:294:ALA:H	2.17	0.46
1:B:97:ILE:HD13	1:B:222:ARG:HG2	1.98	0.46
1:A:171:CYS:SG	1:A:242:LEU:HD22	2.55	0.46
1:A:212:ARG:HH12	1:A:216:ARG:NH2	2.13	0.46
1:A:189:ALA:HA	1:B:130:MET:HG2	1.97	0.46
1:B:58:HIS:CD2	1:B:58:HIS:H	2.34	0.46
1:A:69:LEU:HD11	1:A:340:LEU:CG	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:O	1:A:304:LEU:HD23	2.15	0.45
1:B:212:ARG:HD3	1:B:212:ARG:O	2.17	0.45
1:B:53:TYR:CG	1:B:164:HIS:HD2	2.34	0.45
1:A:164:HIS:CG	1:A:165:PRO:CD	3.00	0.45
1:B:142:HIS:HD2	1:B:357:SER:OG	2.00	0.45
1:A:116:ASP:O	1:A:119:VAL:HG12	2.17	0.45
1:A:194:ILE:O	1:A:318:ARG:HD2	2.16	0.45
1:A:204:VAL:HA	1:A:325:PHE:O	2.16	0.45
1:A:213:HIS:HD2	1:A:213:HIS:O	1.99	0.45
1:A:84:PRO:HG3	1:A:131:PRO:HB2	1.99	0.45
1:B:184:PRO:HB2	1:B:297:LEU:HD11	1.98	0.44
1:B:121:MET:HG3	1:B:181:SER:HB2	1.98	0.44
1:A:299:ALA:N	1:A:303:ASP:O	2.39	0.44
1:B:323:HIS:CE1	1:B:348:VAL:HG21	2.52	0.44
1:B:63:THR:HG22	1:B:162:ASP:OD2	2.18	0.44
1:B:163:ARG:NH2	1:B:172:TYR:HE2	2.16	0.44
1:B:164:HIS:CG	1:B:165:PRO:HD2	2.53	0.44
1:B:97:ILE:CD1	1:B:222:ARG:HG2	2.47	0.44
1:A:221:GLN:N	4:A:714:HOH:O	2.50	0.44
1:B:57:PRO:HB2	1:B:213:HIS:HE1	1.82	0.44
1:B:327:LEU:HD23	1:B:329:TYR:OH	2.17	0.44
1:B:248:TYR:CE1	1:B:253:GLY:HA3	2.53	0.44
1:B:167:ALA:HB3	3:B:2:BTD:BR	2.72	0.44
1:A:169:LEU:HD23	1:A:190:PHE:HD1	1.83	0.44
1:A:167:ALA:HA	1:A:171:CYS:HB2	1.99	0.44
1:A:58:HIS:H	1:A:58:HIS:HD2	1.63	0.43
1:A:130:MET:HB3	1:A:131:PRO:HD3	1.98	0.43
1:A:367:THR:HG23	1:A:370:ARG:NH2	2.33	0.43
1:A:313:ASP:O	1:A:317:LYS:HB2	2.18	0.43
1:A:352:VAL:HB	1:A:357:SER:CB	2.48	0.43
1:A:352:VAL:HB	1:A:357:SER:HB2	2.00	0.43
1:A:215:ASP:O	1:A:218:ALA:HB3	2.18	0.43
1:A:87:TYR:CD1	1:A:91:LEU:HB2	2.54	0.43
1:B:102:THR:O	1:B:106:ARG:N	2.50	0.43
1:B:125:GLN:HG3	1:B:182:MET:CE	2.48	0.43
1:B:256:ARG:HG2	1:B:256:ARG:NH1	2.34	0.43
1:A:119:VAL:HG13	1:A:120:VAL:N	2.34	0.43
1:B:89:ARG:HD3	4:B:530:HOH:O	2.18	0.43
1:A:372:MET:SD	1:B:307:VAL:CG1	3.07	0.42
1:B:124:ALA:O	1:B:128:MET:HG2	2.19	0.42
1:A:283:HIS:C	1:A:285:GLY:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:HIS:O	1:A:285:GLY:N	2.52	0.42
1:A:371:GLU:OE1	1:B:306:ASN:HB2	2.18	0.42
1:A:87:TYR:HA	1:A:91:LEU:CB	2.41	0.42
1:B:54:ILE:HD12	1:B:54:ILE:N	2.34	0.42
1:A:58:HIS:HE1	4:A:576:HOH:O	2.03	0.42
1:A:164:HIS:O	3:A:1:BTD:BR	2.93	0.42
1:A:174:ALA:O	1:A:177:TYR:HB3	2.19	0.42
1:A:62:LYS:HB3	4:A:679:HOH:O	2.19	0.42
1:B:101:TYR:CE2	1:B:225:GLU:HG3	2.55	0.42
1:A:50:LEU:HD13	1:A:52:VAL:CG2	2.50	0.42
1:A:135:THR:O	1:A:139:LEU:HB2	2.19	0.42
1:B:146:GLU:HA	1:B:350:THR:HA	2.02	0.42
1:A:332:SER:O	1:A:335:GLY:N	2.53	0.42
1:A:58:HIS:CD2	1:A:172:TYR:OH	2.73	0.41
1:A:341:LEU:O	1:A:344:THR:HB	2.20	0.41
1:A:213:HIS:O	1:A:213:HIS:CD2	2.73	0.41
1:A:138:VAL:HG13	4:A:593:HOH:O	2.20	0.41
1:A:217:LEU:CD1	1:A:232:LEU:HG	2.48	0.41
1:B:235:ILE:HA	1:B:235:ILE:HD12	1.81	0.41
1:A:178:LEU:HD11	1:A:291:LEU:HD22	2.03	0.41
1:B:301:ASN:C	1:B:301:ASN:OD1	2.59	0.41
1:A:178:LEU:HD12	1:A:178:LEU:HA	1.83	0.40
1:A:198:LEU:HD21	4:A:723:HOH:O	2.22	0.40
1:A:294:ALA:HA	1:A:295:PRO:HD2	1.91	0.40
1:A:62:LYS:NZ	4:A:657:HOH:O	2.55	0.40
1:A:58:HIS:CD2	1:A:58:HIS:N	2.87	0.40
1:A:61:GLY:O	1:A:65:THR:CG2	2.69	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)
4:A:580:HOH:O	4:B:634:HOH:O[6_565]	1.60	0.60

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	295/331 (89%)	273 (92%)	21 (7%)	1 (0%)	46	54
1	B	299/331 (90%)	278 (93%)	21 (7%)	0	100	100
All	All	594/662 (90%)	551 (93%)	42 (7%)	1 (0%)	52	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ILE

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	241/264 (91%)	221 (92%)	20 (8%)	14	14
1	B	242/264 (92%)	217 (90%)	25 (10%)	9	8
All	All	483/528 (92%)	438 (91%)	45 (9%)	11	10

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	65	THR
1	A	94	SER
1	A	121	MET
1	A	130	MET
1	A	173	PRO
1	A	178	LEU
1	A	212	ARG
1	A	216	ARG
1	A	217	LEU
1	A	219	LYS

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Mol	Chain	Res	Type
1	A	220	ARG
1	A	227	LEU
1	A	232	LEU
1	A	293	ARG
1	A	300	PRO
1	A	304	LEU
1	A	307	VAL
1	A	341	LEU
1	A	353	THR
1	B	55	ASP
1	B	85	MET
1	B	107	LEU
1	B	109	GLN
1	B	123	SER
1	B	165	PRO
1	B	173	PRO
1	B	178	LEU
1	B	182	MET
1	B	210	GLU
1	B	212	ARG
1	B	217	LEU
1	B	219	LYS
1	B	222	ARG
1	B	232	LEU
1	B	281	ARG
1	B	293	ARG
1	B	301	ASN
1	B	304	LEU
1	B	307	VAL
1	B	341	LEU
1	B	342	GLN
1	B	344	THR
1	B	354	THR
1	B	364	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	109	GLN
1	A	142	HIS
1	A	323	HIS

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Mol	Chain	Res	Type
1	A	351	HIS
1	B	58	HIS
1	B	142	HIS
1	B	164	HIS
1	B	221	GLN
1	B	323	HIS
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 carbohydrates 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	BTD	A	1	-	18,24,24	3.88	5 (27%)	14,35,35	3.28	4 (28%)
2	SO4	A	3	-	4,4,4	1.46	1 (25%)	6,6,6	0.44	0
3	BTD	B	2	-	18,24,24	2.36	6 (33%)	14,35,35	3.47	6 (42%)
2	SO4	B	4	-	4,4,4	1.27	0	6,6,6	0.95	1 (16%)

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	BTD	A	1	-	-	0/2/22/22	0/3/3/3
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0
3	BTD	B	2	-	-	0/2/22/22	0/3/3/3
2	SO4	B	4	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	BTD	C5-C55	-14.66	1.33	1.48
3	B	2	BTD	C5-C55	-6.23	1.42	1.48
3	A	1	BTD	C6-C5	-4.41	1.29	1.38
3	B	2	BTD	O3'-C3'	-3.40	1.35	1.43
3	B	2	BTD	C3'-C4'	-3.04	1.44	1.53
3	B	2	BTD	C5'-C4'	-2.31	1.43	1.51
3	B	2	BTD	C2'-C1'	-2.26	1.46	1.52
2	A	3	SO4	O2-S	-2.01	1.40	1.47
3	A	1	BTD	C4-N3	2.75	1.38	1.33
3	A	1	BTD	O4'-C1'	2.82	1.48	1.42
3	A	1	BTD	C22-S11	3.29	1.78	1.72
3	B	2	BTD	C6-N1	3.62	1.40	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2	BTD	O4'-C1'-N1	-4.07	100.68	107.72
3	A	1	BTD	C5'-C4'-C3'	-2.70	107.61	114.80
3	B	2	BTD	O3'-C3'-C4'	-2.39	100.41	110.05
3	B	2	BTD	O4'-C1'-C2'	-2.20	101.89	106.27
3	B	2	BTD	O4'-C4'-C5'	-2.15	104.52	109.17
2	B	4	SO4	O2-S-O1	-2.02	103.10	109.50
3	B	2	BTD	C3'-C2'-C1'	2.16	107.58	102.40
3	A	1	BTD	C2'-C1'-N1	2.43	120.06	114.16
3	A	1	BTD	O4'-C4'-C5'	2.46	114.50	109.17
3	A	1	BTD	C4-N3-C2	10.71	124.51	115.25
3	B	2	BTD	C4-N3-C2	10.88	124.65	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	BTD	3	0
3	B	2	BTD	5	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	303/331 (91%)	-0.39	1 (0%)	94	97	6, 18, 34, 46	0
1	B	307/331 (92%)	-0.38	3 (0%)	84	91	4, 18, 34, 40	0
All	All	610/662 (92%)	-0.38	4 (0%)	89	93	4, 18, 34, 46	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ARG	3.8
1	B	222	ARG	2.1
1	B	221	GLN	2.0
1	B	300	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	4	5/5	0.99	0.10	-0.67	37,39,41,42	0
3	BTD	B	2	22/22	0.97	0.08	-0.69	10,15,23,31	0
3	BTD	A	1	22/22	0.98	0.08	-1.10	11,15,25,26	0
2	SO4	A	3	5/5	0.99	0.05	-1.66	20,21,22,22	0

6.5 Other polymers (i)

There are no such residues in this entry.