



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:34 PM UTC

PDB ID : 2A2A / pdb_00002a2a
Title : High-resolution crystallographic analysis of the autoinhibited conformation of a human death-associated protein kinase
Authors : Kursula, P.; Wilmanns, M.
Deposited on : 2005-06-22
Resolution : 1.47 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)
Xtrriage (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

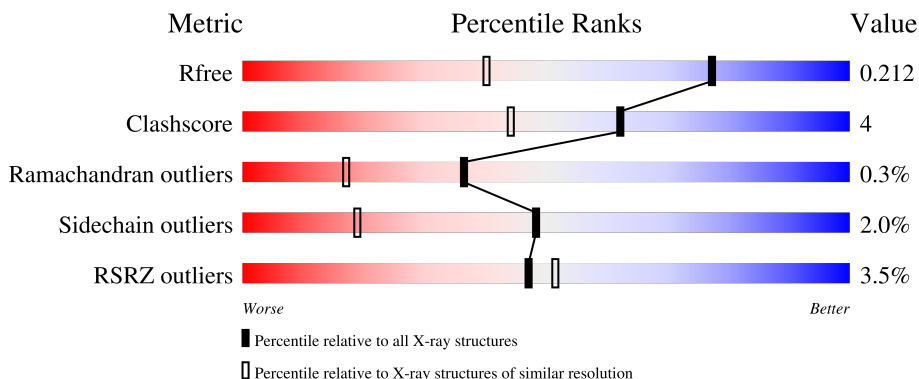
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	321	 3% 86% 8% • 5%
1	B	321	 4% 85% 8% • 6%
1	C	321	 3% 85% 8% • 6%
1	D	321	 3% 87% 7% • 6%

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
4	DTT	A	2002	X	-	-	-
4	DTT	B	2003	X	-	-	-
4	DTT	C	2004	X	-	-	-
4	DTT	D	2005	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11556 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 Death-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	304	Total 2557	C 1628	N 436	O 488	S 5	0	10	0
1	B	303	Total 2523	C 1609	N 434	O 476	S 4	0	7	0
1	C	303	Total 2532	C 1619	N 431	O 478	S 4	0	8	0
1	D	303	Total 2512	C 1605	N 433	O 470	S 4	0	5	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q9UIK4
A	231	SER	ALA	SEE REMARK 999	UNP Q9UIK4
A	243	HIS	GLN	SEE REMARK 999	UNP Q9UIK4
B	0	GLY	-	expression tag	UNP Q9UIK4
B	231	SER	ALA	SEE REMARK 999	UNP Q9UIK4
B	243	HIS	GLN	SEE REMARK 999	UNP Q9UIK4
C	0	GLY	-	expression tag	UNP Q9UIK4
C	231	SER	ALA	SEE REMARK 999	UNP Q9UIK4
C	243	HIS	GLN	SEE REMARK 999	UNP Q9UIK4
D	0	GLY	-	expression tag	UNP Q9UIK4
D	231	SER	ALA	SEE REMARK 999	UNP Q9UIK4
D	243	HIS	GLN	SEE REMARK 999	UNP Q9UIK4

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Na 2	0	0
2	B	2	Total 2	Na 2	0	0

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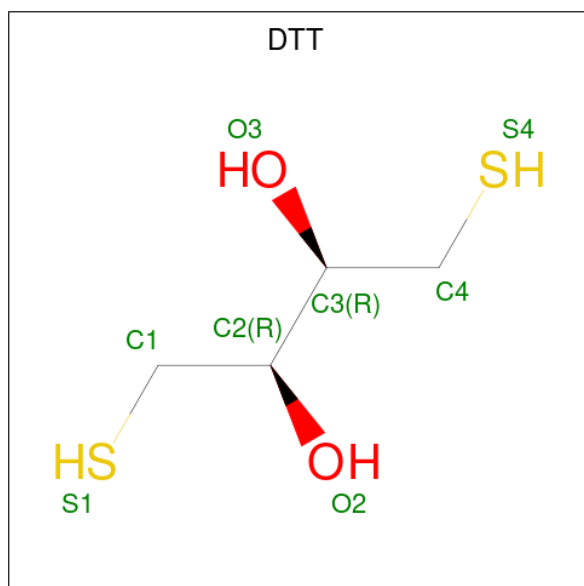
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	3	Total	Na	0	0
			3	3		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			8	4	2	2		
4	B	1	Total	C	O	S	0	0
			8	4	2	2		
4	C	1	Total	C	O	S	0	0
			8	4	2	2		
4	D	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

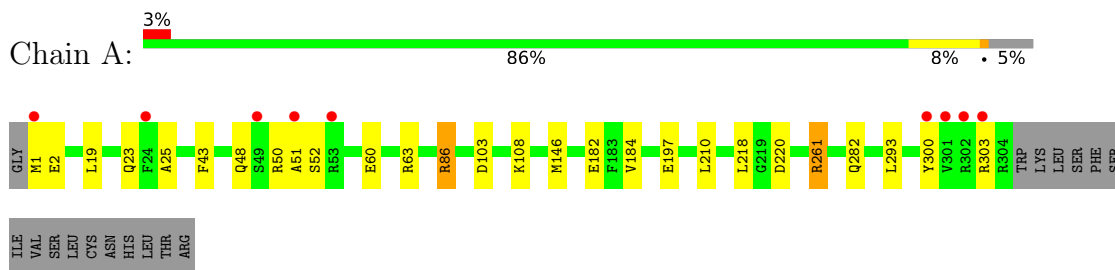
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	361	Total O 361 361	0	0
6	B	315	Total O 315 315	0	0
6	C	346	Total O 346 346	0	0
6	D	349	Total O 349 349	0	0

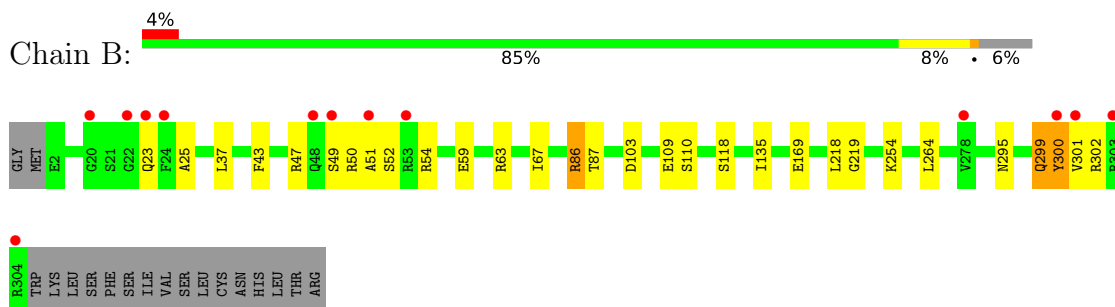
3 Residue-property plots [i](#)

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.

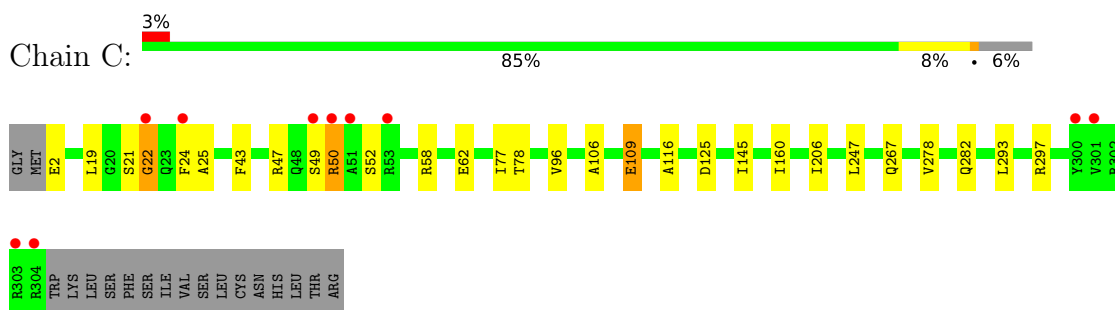
- Molecule 1: Death-associated protein kinase 2



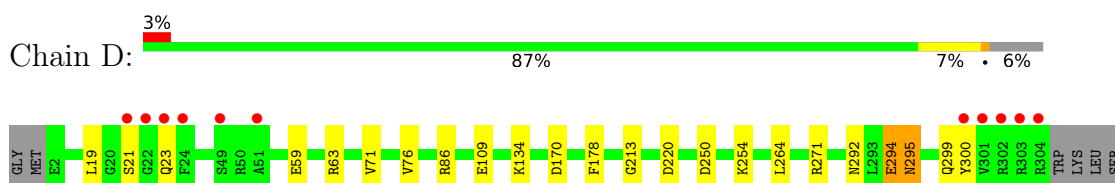
- Molecule 1: Death-associated protein kinase 2



- Molecule 1: Death-associated protein kinase 2



- Molecule 1: Death-associated protein kinase 2



PHE
SER
ILE
VAL
SER
LEU
CYS
ASN
HIS
LEU
THR
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.30Å 60.65Å 98.71Å 92.16° 103.45° 94.25°	Depositor
Resolution (Å)	20.00 – 1.47 20.00 – 1.47	Depositor EDS
% Data completeness (in resolution range)	94.8 (20.00-1.47) 94.8 (20.00-1.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.47Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.150 , 0.207 0.153 , 0.212	Depositor DCC
R_{free} test set	2004 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtrriage
Anisotropy	0.102	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 67.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11556	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DTT, CL, NA, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.00	0/2605	0.94	1/3513 (0.0%)
1	B	0.96	0/2571	0.92	0/3466
1	C	0.98	1/2580 (0.0%)	0.94	2/3480 (0.1%)
1	D	1.00	0/2560	0.94	0/3452
All	All	0.99	1/10316 (0.0%)	0.94	3/13911 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	116	ALA	CA-CB	-5.62	1.44	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	VAL	N-CA-C	5.35	116.48	109.21
1	C	2	GLU	CA-C-N	-5.17	114.62	119.85
1	C	2	GLU	C-N-CA	-5.17	114.62	119.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2557	0	2541	27	0
1	B	2523	0	2523	23	0
1	C	2532	0	2535	15	0
1	D	2512	0	2520	23	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	1	0
3	C	1	0	0	0	0
4	A	8	0	8	2	0
4	B	8	0	8	0	0
4	C	8	0	8	0	0
4	D	8	0	8	0	0
5	A	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	361	0	0	9	0
6	B	315	0	0	5	0
6	C	346	0	0	6	0
6	D	349	0	0	5	0
All	All	11556	0	10175	84	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 4.

All (84) 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)
4:A:2002:DTT:S1	4:A:2002:DTT:S4	2.29	1.30
1:D:71[A]:VAL:HG11	1:D:76:VAL:HG11	1.38	1.05
1:A:23:GLN:N	6:A:3645:HOH:O	2.08	0.85
1:C:109:GLU:H	1:C:109:GLU:CD	1.91	0.76
1:D:71[A]:VAL:HG11	1:D:76:VAL:CG1	2.16	0.75
1:D:292:ASN:HB3	1:D:295:ASN:HD21	1.53	0.71
1:C:78[A]:THR:HG22	6:C:3307:HOH:O	1.95	0.67
1:B:299:GLN:HE21	1:B:299:GLN:HA	1.59	0.67
1:D:292:ASN:CG	1:D:295:ASN:HD21	2.03	0.66
1:D:292:ASN:CB	1:D:295:ASN:HD21	2.09	0.65
1:D:295:ASN:O	1:D:299:GLN:HG2	1.96	0.65
1:D:59:GLU:OE2	6:D:3512:HOH:O	2.15	0.65
1:D:292:ASN:HB3	1:D:295:ASN:ND2	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ARG:HD3	6:A:3618:HOH:O	1.98	0.63
6:C:3598:HOH:O	1:D:220:ASP:HB2	1.97	0.63
1:B:110[A]:SER:OG	6:B:3920:HOH:O	2.16	0.62
1:C:77[B]:ILE:HD13	1:C:160:ILE:HG22	1.81	0.62
1:D:250:ASP:OD2	6:D:3476:HOH:O	2.16	0.61
1:D:271:ARG:HG3	6:D:3467:HOH:O	2.01	0.61
1:D:295:ASN:ND2	1:D:295:ASN:H	1.99	0.60
1:C:125:ASP:OD2	6:C:3605:HOH:O	2.17	0.59
1:A:218:LEU:CD2	1:B:51:ALA:HB2	2.33	0.59
1:A:63[A]:ARG:HD3	3:A:3065:CL:CL	2.40	0.58
1:A:182:GLU:OE1	1:A:303:ARG:NH2	2.37	0.57
1:A:108:LYS:HE3	6:A:3627:HOH:O	2.05	0.56
1:B:118[B]:SER:O	6:B:3930:HOH:O	2.18	0.56
1:A:218:LEU:HD21	1:B:51:ALA:HB2	1.87	0.55
1:B:299:GLN:HE22	1:B:302:ARG:NH1	2.05	0.54
1:B:63[A]:ARG:NH1	6:B:4051:HOH:O	2.39	0.54
1:B:109:GLU:HB2	6:B:3911:HOH:O	2.07	0.54
1:A:60:GLU:HG2	1:A:63[B]:ARG:NH2	2.23	0.53
1:B:103:ASP:OD2	1:B:300:TYR:HE1	1.92	0.53
1:A:108:LYS:CE	6:A:3627:HOH:O	2.56	0.53
1:A:220:ASP:HB2	6:A:3635:HOH:O	2.08	0.52
1:D:213:GLY:O	1:D:299:GLN:HG3	2.09	0.51
1:A:86:ARG:H	1:A:86:ARG:HD2	1.75	0.51
1:B:59:GLU:HG2	1:B:63[B]:ARG:NH2	2.26	0.51
1:A:303:ARG:HG2	1:B:51:ALA:O	2.11	0.50
1:A:50:ARG:HH21	1:B:219:GLY:HA2	1.77	0.49
1:A:197[A]:GLU:H	1:A:197[A]:GLU:CD	2.20	0.49
1:D:294:GLU:OE2	1:D:294:GLU:HA	2.12	0.49
1:A:86:ARG:HD2	1:A:86:ARG:N	2.27	0.49
1:A:86:ARG:H	1:A:86:ARG:CD	2.25	0.49
1:A:282:GLN:HB3	6:A:3614:HOH:O	2.12	0.49
1:A:103:ASP:HB2	1:A:300:TYR:OH	2.12	0.49
1:B:103:ASP:OD2	1:B:300:TYR:CE1	2.66	0.49
1:C:58:ARG:NE	1:C:62:GLU:OE1	2.40	0.49
1:C:106:ALA:O	1:C:297:ARG:NE	2.43	0.48
1:A:25:ALA:HA	1:A:43:PHE:O	2.13	0.48
1:C:24:PHE:C	6:C:3610:HOH:O	2.55	0.48
1:C:25:ALA:HA	1:C:43:PHE:O	2.14	0.47
1:A:261:ARG:NE	6:A:3371:HOH:O	2.24	0.47
1:A:50:ARG:N	6:A:3620:HOH:O	2.48	0.47
4:A:2002:DTT:S1	4:A:2002:DTT:C4	3.01	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ALA:N	6:C:3610:HOH:O	2.47	0.47
1:D:292:ASN:CG	1:D:295:ASN:ND2	2.73	0.46
1:C:278:VAL:HG22	1:C:282:GLN:OE1	2.15	0.46
1:D:134:LYS:NZ	1:D:170:ASP:OD2	2.49	0.46
1:D:86:ARG:HG3	6:D:3444:HOH:O	2.16	0.46
1:D:292:ASN:CB	1:D:295:ASN:ND2	2.77	0.45
1:A:146:MET:CE	6:A:3495:HOH:O	2.64	0.45
1:C:247:LEU:HD12	6:C:3633:HOH:O	2.17	0.44
1:B:49:SER:N	1:B:52:SER:OG	2.50	0.44
1:A:1:MET:O	1:A:2:GLU:C	2.60	0.44
1:C:145[A]:ILE:HD11	1:C:206:ILE:HD13	1.99	0.44
1:B:295:ASN:O	1:B:299:GLN:HG2	2.18	0.43
1:B:109:GLU:O	6:B:4041:HOH:O	2.21	0.43
1:C:77[B]:ILE:CD1	1:C:96:VAL:HG21	2.49	0.42
1:D:59:GLU:HG2	1:D:63[B]:ARG:NH2	2.34	0.42
1:D:71[A]:VAL:CG1	1:D:76:VAL:HG11	2.28	0.42
1:A:210:LEU:C	1:A:210:LEU:HD23	2.44	0.42
1:B:67:ILE:HG23	1:B:135:ILE:HD13	2.01	0.42
1:D:109:GLU:HG2	6:D:3297:HOH:O	2.20	0.42
1:D:254:LYS:HB3	1:D:264:LEU:HG	2.02	0.42
1:B:47:ARG:CZ	1:B:50:ARG:HA	2.50	0.42
1:C:47:ARG:HG3	1:C:52:SER:HB2	2.02	0.41
1:A:51:ALA:HB2	1:B:218:LEU:CD2	2.50	0.41
1:B:86:ARG:HD2	1:B:87[B]:THR:HG23	2.01	0.41
1:C:21:SER:O	1:C:22:GLY:O	2.38	0.41
1:A:48:GLN:HB2	1:A:52:SER:OG	2.21	0.40
1:A:218:LEU:HD22	1:B:51:ALA:HB2	2.01	0.40
1:B:254[B]:LYS:HB3	1:B:264:LEU:HG	2.03	0.40
1:B:25:ALA:HA	1:B:43:PHE:O	2.21	0.40
1:D:178:PHE:CD1	1:D:178:PHE:C	2.99	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	312/321 (97%)	303 (97%)	9 (3%)	0	100	100
1	B	308/321 (96%)	298 (97%)	9 (3%)	1 (0%)	36	17
1	C	309/321 (96%)	295 (96%)	12 (4%)	2 (1%)	21	6
1	D	306/321 (95%)	298 (97%)	7 (2%)	1 (0%)	36	17
All	All	1235/1284 (96%)	1194 (97%)	37 (3%)	4 (0%)	36	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	GLN
1	C	22	GLY
1	C	50	ARG
1	D	21	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	283/290 (98%)	279 (99%)	4 (1%)	59	31
1	B	279/290 (96%)	272 (98%)	7 (2%)	42	13
1	C	280/290 (97%)	274 (98%)	6 (2%)	47	17
1	D	277/290 (96%)	272 (98%)	5 (2%)	51	22
All	All	1119/1160 (96%)	1097 (98%)	22 (2%)	48	19

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	86	ARG
1	A	261	ARG
1	A	293	LEU

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Mol	Chain	Res	Type
1	B	37	LEU
1	B	54	ARG
1	B	86	ARG
1	B	169	GLU
1	B	299	GLN
1	B	300	TYR
1	B	301	VAL
1	C	19	LEU
1	C	49	SER
1	C	50	ARG
1	C	109	GLU
1	C	267	GLN
1	C	293	LEU
1	D	19	LEU
1	D	23	GLN
1	D	294	GLU
1	D	295	ASN
1	D	300	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	228	ASN
1	A	295	ASN
1	B	48	GLN
1	B	166	HIS
1	B	223	GLN
1	B	280	ASN
1	B	295	ASN
1	B	299	GLN
1	C	23	GLN
1	C	128	ASN
1	C	166	HIS
1	C	243	HIS
1	C	267	GLN
1	D	223	GLN
1	D	295	ASN

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](#)

Of 18 ligands modelled in this entry, 11 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	C	3002	-	5,5,5	0.47	0	5,5,5	0.93	0
4	DTT	D	2005	-	7,7,7	0.68	0	4,8,8	1.14	0
5	GOL	D	3003	-	5,5,5	0.38	0	5,5,5	0.90	0
5	GOL	A	3001	-	5,5,5	0.28	0	5,5,5	0.53	0
4	DTT	A	2002	-	7,7,7	1.07	0	4,8,8	0.74	0
4	DTT	B	2003	-	7,7,7	0.82	0	4,8,8	1.50	1 (25%)
4	DTT	C	2004	-	7,7,7	0.87	0	4,8,8	1.70	2 (50%)

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
5	GOL	C	3002	-	-	4/4/4/4	-
4	DTT	D	2005	-	1/1/2/2	7/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	D	3003	-	-	2/4/4/4	-
5	GOL	A	3001	-	-	2/4/4/4	-
4	DTT	A	2002	-	1/1/2/2	4/8/8/8	-
4	DTT	B	2003	-	1/1/2/2	4/8/8/8	-
4	DTT	C	2004	-	1/1/2/2	4/8/8/8	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2003	DTT	C2-C1-S1	-2.24	108.17	114.43
4	C	2004	DTT	O2-C2-C3	2.16	114.11	109.57
4	C	2004	DTT	O3-C3-C2	2.02	113.82	109.57

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	2002	DTT	C3
4	B	2003	DTT	C3
4	C	2004	DTT	C3
4	D	2005	DTT	C3

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2002	DTT	C1-C2-C3-O3
4	A	2002	DTT	C1-C2-C3-C4
4	A	2002	DTT	O2-C2-C3-O3
4	A	2002	DTT	O2-C2-C3-C4
4	B	2003	DTT	C1-C2-C3-O3
4	B	2003	DTT	C1-C2-C3-C4
4	B	2003	DTT	O2-C2-C3-O3
4	B	2003	DTT	O2-C2-C3-C4
4	C	2004	DTT	C1-C2-C3-O3
4	C	2004	DTT	C1-C2-C3-C4
4	C	2004	DTT	O2-C2-C3-O3
4	C	2004	DTT	O2-C2-C3-C4
4	D	2005	DTT	S1-C1-C2-C3
4	D	2005	DTT	C1-C2-C3-O3
4	D	2005	DTT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	D	2005	DTT	O2-C2-C3-O3
4	D	2005	DTT	O2-C2-C3-C4
4	D	2005	DTT	C2-C3-C4-S4
5	C	3002	GOL	C1-C2-C3-O3
5	A	3001	GOL	O1-C1-C2-C3
5	C	3002	GOL	O1-C1-C2-C3
5	D	3003	GOL	O1-C1-C2-C3
5	C	3002	GOL	O2-C2-C3-O3
4	D	2005	DTT	O3-C3-C4-S4
5	A	3001	GOL	O1-C1-C2-O2
5	D	3003	GOL	O1-C1-C2-O2
5	C	3002	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	DTT	2	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	304/321 (94%)	-0.10	9 (2%) 52 57	9, 23, 52, 76	10 (3%)
1	B	303/321 (94%)	-0.04	13 (4%) 40 44	9, 23, 54, 83	7 (2%)
1	C	303/321 (94%)	-0.09	10 (3%) 49 53	8, 23, 48, 73	8 (2%)
1	D	303/321 (94%)	-0.05	11 (3%) 46 50	9, 22, 47, 93	5 (1%)
All	All	1213/1284 (94%)	-0.07	43 (3%) 47 51	8, 23, 52, 93	30 (2%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	51	ALA	5.2
1	D	300	TYR	5.2
1	A	51	ALA	4.2
1	B	24	PHE	4.2
1	D	301	VAL	4.1
1	B	300	TYR	3.8
1	B	301	VAL	3.6
1	D	303	ARG	3.5
1	D	24	PHE	3.5
1	C	51	ALA	3.5
1	C	24	PHE	3.3
1	A	24	PHE	3.2
1	A	49	SER	3.0
1	B	303	ARG	2.9
1	D	51	ALA	2.8
1	B	48	GLN	2.8
1	B	304	ARG	2.8
1	D	21	SER	2.7
1	C	300	TYR	2.6
1	D	22	GLY	2.6
1	B	22	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	300	TYR	2.5
1	C	22	GLY	2.5
1	C	301	VAL	2.5
1	D	49	SER	2.4
1	D	304	ARG	2.4
1	A	301	VAL	2.4
1	C	304	ARG	2.4
1	B	23	GLN	2.3
1	B	20	GLY	2.3
1	A	1	MET	2.3
1	A	303	ARG	2.2
1	B	278	VAL	2.2
1	A	53	ARG	2.1
1	C	303	ARG	2.1
1	C	49	SER	2.1
1	A	302	ARG	2.1
1	C	50	ARG	2.1
1	D	23	GLN	2.1
1	B	49	SER	2.1
1	C	53	ARG	2.0
1	D	302	ARG	2.0
1	B	53	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(\AA^2)	Q<0.9
4	DTT	A	2002	8/8	0.88	0.12	39,43,49,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NA	B	3763	1/1	0.91	0.12	52,52,52,52	0
4	DTT	C	2004	8/8	0.91	0.11	39,42,42,46	0
5	GOL	A	3001	6/6	0.91	0.08	26,33,36,37	0
4	DTT	D	2005	8/8	0.92	0.10	42,47,51,54	0
2	NA	C	3281	1/1	0.92	0.13	66,66,66,66	0
5	GOL	C	3002	6/6	0.92	0.08	27,36,38,41	0
4	DTT	B	2003	8/8	0.93	0.10	35,41,48,50	0
2	NA	C	3158	1/1	0.95	0.13	31,31,31,31	0
3	CL	A	3318	1/1	0.95	0.08	53,53,53,53	0
5	GOL	D	3003	6/6	0.95	0.07	25,32,38,44	0
2	NA	A	3178	1/1	0.96	0.18	43,43,43,43	0
2	NA	B	3221	1/1	0.96	0.16	40,40,40,40	0
2	NA	C	3291	1/1	0.96	0.14	46,46,46,46	0
2	NA	D	3175	1/1	0.96	0.13	46,46,46,46	0
3	CL	C	3039	1/1	0.98	0.12	38,38,38,38	0
2	NA	A	3152	1/1	0.98	0.08	32,32,32,32	0
3	CL	A	3065	1/1	0.99	0.08	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.