



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:14 AM UTC

PDB ID : 2A27 / pdb_00002a27
Title : Human DRP-1 kinase, W305S S308A D40 mutant, crystal form with 8 monomers in the asymmetric unit
Authors : Kursula, P.; Lehmann, F.; Shani, G.; Kimchi, A.; Wilmanns, M.
Deposited on : 2005-06-22
Resolution : 3.00 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:

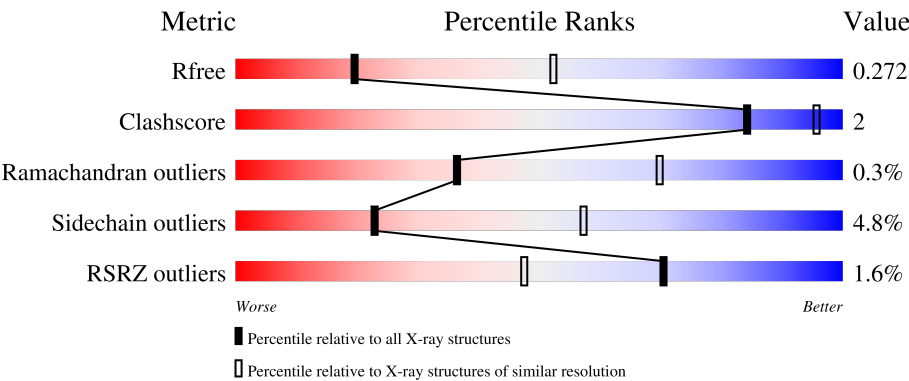
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	2% 84%9%• 5%
1	B	321	2% 85%7%• 6%
1	C	321	2% 84%8%• 6%
1	D	321	2% 86%8%• 5%
1	E	321	3% 87%7%• 6%

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Mol	Chain	Length	Quality of chain
1	F	321	 86% 7% • 6%
1	G	321	 86% 7% • 6%
1	H	321	 86% 8% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTT	A	1001	X	-	-	-
2	DTT	B	1002	X	-	-	-
2	DTT	C	1003	X	-	-	-
2	DTT	D	1004	X	-	-	-
2	DTT	E	1005	X	-	-	-
2	DTT	F	1007	X	-	-	-
2	DTT	G	1006	X	-	-	-
2	DTT	H	1008	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20003 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
1	A	304	Total	C	N	O	S	0	0	0
			2478	1584	425	465	4			
1	B	303	Total	C	N	O	S	0	0	0
			2467	1578	421	464	4			
1	C	303	Total	C	N	O	S	0	0	0
			2467	1578	421	464	4			
1	D	304	Total	C	N	O	S	0	0	0
			2478	1584	425	465	4			
1	E	303	Total	C	N	O	S	0	0	0
			2467	1578	421	464	4			
1	F	303	Total	C	N	O	S	0	0	0
			2467	1578	421	464	4			
1	G	303	Total	C	N	O	S	0	0	0
			2467	1578	421	464	4			
1	H	304	Total	C	N	O	S	0	0	0
			2472	1581	422	465	4			

There are 24 discrepancies between the modelled and reference sequences:

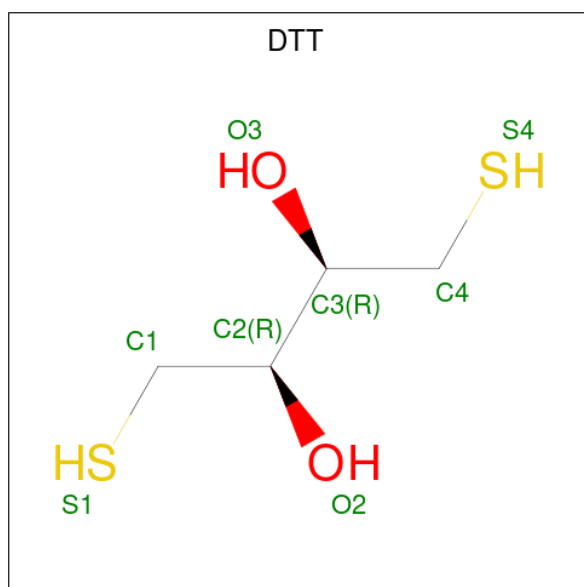
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP Q9UIK4
A	305	SER	TRP	engineered mutation	UNP Q9UIK4
A	308	ALA	SER	engineered mutation	UNP Q9UIK4
B	0	GLY	-	cloning artifact	UNP Q9UIK4
B	305	SER	TRP	engineered mutation	UNP Q9UIK4
B	308	ALA	SER	engineered mutation	UNP Q9UIK4
C	0	GLY	-	cloning artifact	UNP Q9UIK4
C	305	SER	TRP	engineered mutation	UNP Q9UIK4
C	308	ALA	SER	engineered mutation	UNP Q9UIK4
D	0	GLY	-	cloning artifact	UNP Q9UIK4
D	305	SER	TRP	engineered mutation	UNP Q9UIK4
D	308	ALA	SER	engineered mutation	UNP Q9UIK4
E	0	GLY	-	cloning artifact	UNP Q9UIK4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	305	SER	TRP	engineered mutation	UNP Q9UIK4
E	308	ALA	SER	engineered mutation	UNP Q9UIK4
F	0	GLY	-	cloning artifact	UNP Q9UIK4
F	305	SER	TRP	engineered mutation	UNP Q9UIK4
F	308	ALA	SER	engineered mutation	UNP Q9UIK4
G	0	GLY	-	cloning artifact	UNP Q9UIK4
G	305	SER	TRP	engineered mutation	UNP Q9UIK4
G	308	ALA	SER	engineered mutation	UNP Q9UIK4
H	0	GLY	-	cloning artifact	UNP Q9UIK4
H	305	SER	TRP	engineered mutation	UNP Q9UIK4
H	308	ALA	SER	engineered mutation	UNP Q9UIK4

- Molecule 2 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	F	1	Total	C	O	S	0	0
			8	4	2	2		
2	G	1	Total	C	O	S	0	0
			8	4	2	2		
2	H	1	Total	C	O	S	0	0
			8	4	2	2		

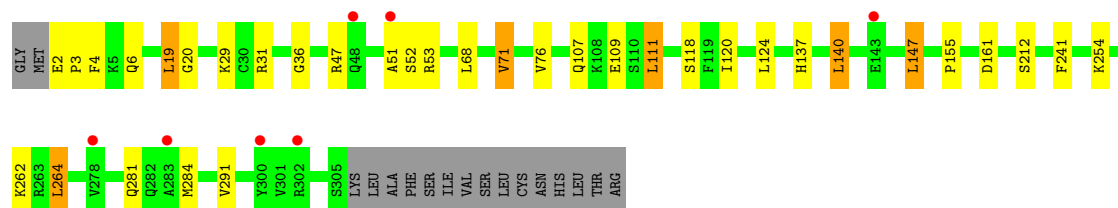
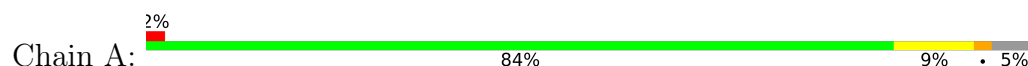
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	55	Total	O	0	0
			55	55		
3	C	44	Total	O	0	0
			44	44		
3	D	17	Total	O	0	0
			17	17		
3	E	9	Total	O	0	0
			9	9		
3	F	3	Total	O	0	0
			3	3		
3	G	5	Total	O	0	0
			5	5		
3	H	6	Total	O	0	0
			6	6		

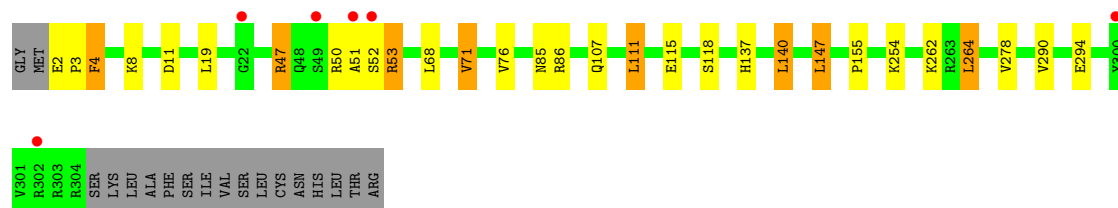
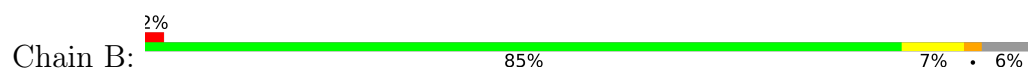
3 Residue-property plots [i](#)

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.

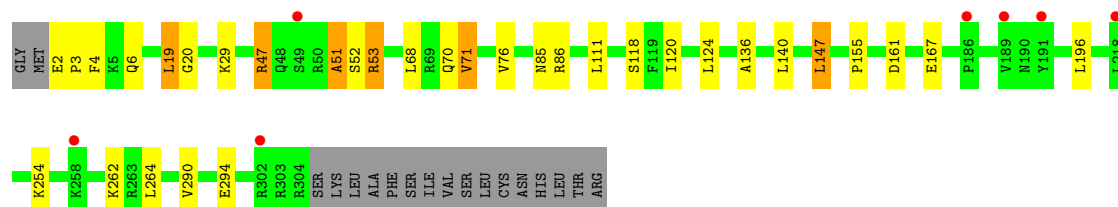
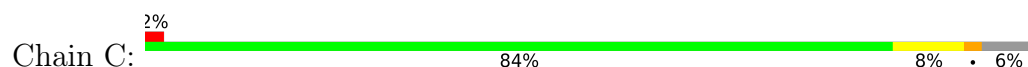
• Molecule 1: Death-associated protein kinase 2



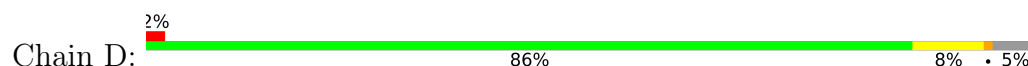
• Molecule 1: Death-associated protein kinase 2

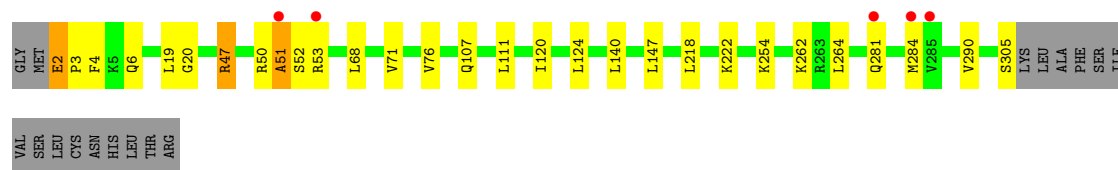


• Molecule 1: Death-associated protein kinase 2

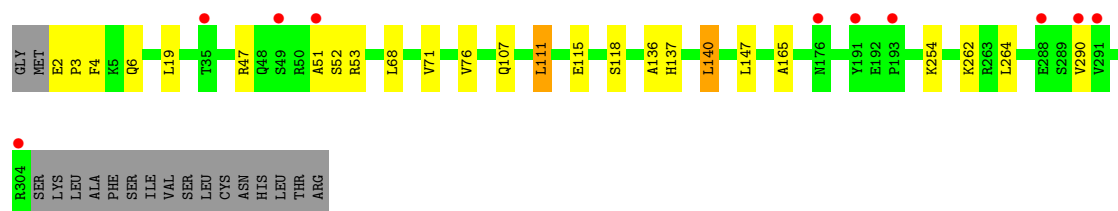
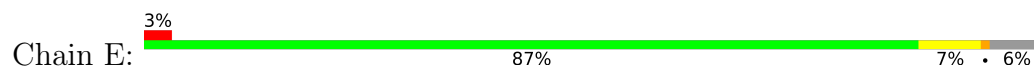


• Molecule 1: Death-associated protein kinase 2

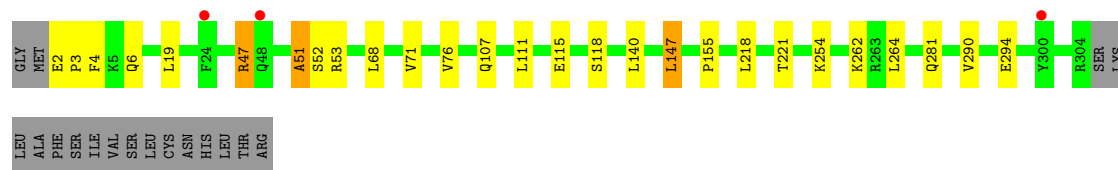
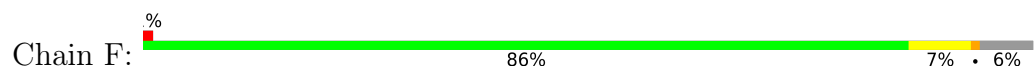




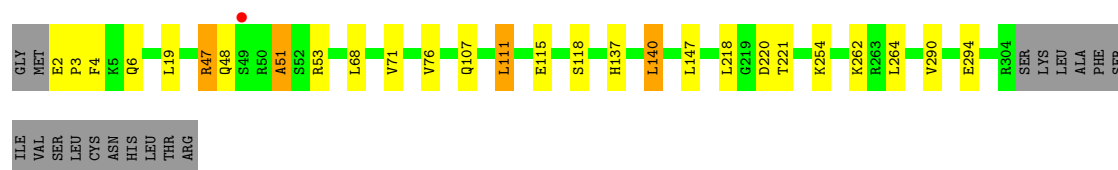
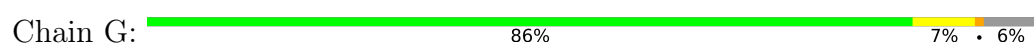
- Molecule 1: Death-associated protein kinase 2



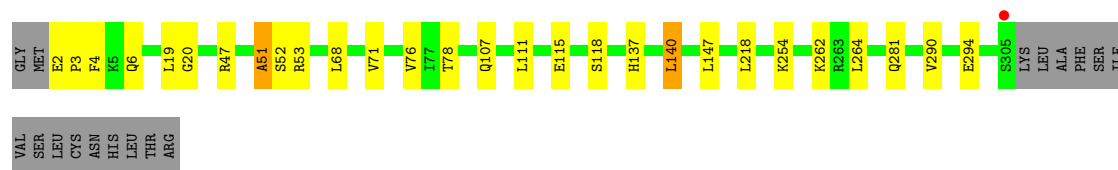
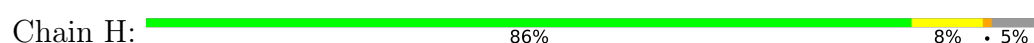
- Molecule 1: Death-associated protein kinase 2



- Molecule 1: Death-associated protein kinase 2



- Molecule 1: Death-associated protein kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.12Å 113.35Å 247.31Å 90.00° 95.09° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 99.5 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.217 , 0.238 (Not available) , 0.272	Depositor DCC
R_{free} test set	4395 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 116.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20003	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.48% 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: DTT

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	0.75	1/2525 (0.0%)	0.92	5/3405 (0.1%)
1	B	0.80	0/2514	0.97	5/3391 (0.1%)
1	C	0.63	0/2514	0.87	5/3391 (0.1%)
1	D	0.57	1/2525 (0.0%)	0.86	2/3405 (0.1%)
1	E	0.51	0/2514	0.84	4/3391 (0.1%)
1	F	0.46	0/2514	0.81	2/3391 (0.1%)
1	G	0.46	0/2514	0.82	3/3391 (0.1%)
1	H	0.47	0/2519	0.82	4/3398 (0.1%)
All	All	0.59	2/20139 (0.0%)	0.86	30/27163 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	2
1	H	0	2
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	MET	SD-CE	8.65	2.01	1.79
1	D	284	MET	SD-CE	5.69	1.93	1.79

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	PRO	N-CA-C	8.06	123.14	111.13
1	D	3	PRO	N-CA-C	7.97	123.00	111.13
1	E	3	PRO	N-CA-C	7.93	125.15	111.03
1	B	3	PRO	N-CA-C	7.74	126.25	112.01
1	H	3	PRO	N-CA-C	7.39	124.19	111.03
1	F	3	PRO	N-CA-C	7.36	122.24	110.40
1	C	3	PRO	N-CA-C	7.20	123.80	111.77
1	G	3	PRO	N-CA-C	7.20	123.85	111.03
1	B	52	SER	N-CA-C	-6.91	97.99	109.46
1	B	278	VAL	N-CA-C	-6.61	105.39	111.67
1	C	3	PRO	CA-C-N	6.60	130.49	121.05
1	C	3	PRO	C-N-CA	6.60	130.49	121.05
1	E	52	SER	N-CA-C	-6.51	98.66	109.46
1	A	3	PRO	CA-C-N	6.47	129.90	120.71
1	A	3	PRO	C-N-CA	6.47	129.90	120.71
1	E	3	PRO	CA-C-N	6.39	129.95	120.87
1	E	3	PRO	C-N-CA	6.39	129.95	120.87
1	A	52	SER	N-CA-C	-6.18	99.16	109.24
1	H	3	PRO	CA-C-N	6.12	129.40	120.71
1	H	3	PRO	C-N-CA	6.12	129.40	120.71
1	G	3	PRO	CA-C-N	6.02	129.38	120.90
1	G	3	PRO	C-N-CA	6.02	129.38	120.90
1	C	52	SER	N-CA-C	-5.95	99.54	109.24
1	H	52	SER	N-CA-C	-5.87	99.62	108.96
1	D	52	SER	N-CA-C	-5.57	100.11	108.96
1	B	3	PRO	CA-C-N	5.48	132.01	121.54
1	B	3	PRO	C-N-CA	5.48	132.01	121.54
1	F	52	SER	N-CA-C	-5.12	100.81	108.96
1	C	71	VAL	N-CA-C	5.08	114.93	107.15
1	A	71	VAL	N-CA-C	5.05	114.88	107.15

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	GLU	Peptide
1	A	51	ALA	Peptide
1	B	2	GLU	Peptide
1	B	51	ALA	Peptide
1	C	2	GLU	Peptide
1	C	51	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	D	2	GLU	Peptide
1	D	51	ALA	Peptide
1	E	2	GLU	Peptide
1	E	51	ALA	Peptide
1	F	2	GLU	Peptide
1	F	51	ALA	Peptide
1	G	2	GLU	Peptide
1	G	51	ALA	Peptide
1	H	2	GLU	Peptide
1	H	51	ALA	Peptide

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	2478	0	2489	13	0
1	B	2467	0	2476	13	0
1	C	2467	0	2476	12	0
1	D	2478	0	2489	16	0
1	E	2467	0	2476	6	0
1	F	2467	0	2476	9	0
1	G	2467	0	2476	15	0
1	H	2472	0	2478	9	0
2	A	8	0	8	2	0
2	B	8	0	8	0	0
2	C	8	0	8	0	0
2	D	8	0	10	0	0
2	E	8	0	8	1	0
2	F	8	0	10	1	0
2	G	8	0	10	1	0
2	H	8	0	10	2	0
3	A	37	0	0	1	0
3	B	55	0	0	3	0
3	C	44	0	0	1	0
3	D	17	0	0	1	0
3	E	9	0	0	0	0
3	F	3	0	0	0	0
3	G	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	6	0	0	1	0
All	All	20003	0	19908	90	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 2.

All (90) 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)
2:A:1001:DTT:S1	2:A:1001:DTT:S4	2.30	1.29
2:E:1005:DTT:S1	2:E:1005:DTT:S4	2.33	1.25
2:H:1008:DTT:HS2	2:H:1008:DTT:HS1	1.21	0.86
2:H:1008:DTT:S1	2:H:1008:DTT:S4	2.83	0.76
1:D:51:ALA:HB3	1:G:218:LEU:HD21	1.72	0.72
1:F:71:VAL:HG11	1:F:76:VAL:HG11	1.74	0.69
2:F:1007:DTT:S1	2:F:1007:DTT:S4	2.73	0.67
3:B:1042:HOH:O	1:C:51:ALA:HB1	1.95	0.66
1:B:4:PHE:HD1	1:B:4:PHE:H	1.44	0.66
1:D:254:LYS:HB3	1:D:264:LEU:HD13	1.80	0.63
1:D:51:ALA:HB2	1:G:218:LEU:HD11	1.82	0.61
1:G:254:LYS:HB3	1:G:264:LEU:HD13	1.83	0.60
1:D:218:LEU:HD21	1:G:51:ALA:HB3	1.82	0.60
1:F:254:LYS:HB3	1:F:264:LEU:HD13	1.82	0.60
1:A:109:GLU:HB2	3:A:1012:HOH:O	2.01	0.59
1:B:254:LYS:HB3	1:B:264:LEU:HD13	1.85	0.58
1:C:85:ASN:HD22	1:C:86:ARG:HD2	1.71	0.56
1:F:218:LEU:HD21	1:H:51:ALA:HB3	1.88	0.56
1:E:71:VAL:HG11	1:E:76:VAL:HG11	1.88	0.55
1:E:254:LYS:HB3	1:E:264:LEU:HD13	1.87	0.55
1:H:254:LYS:HB3	1:H:264:LEU:HD13	1.88	0.54
1:D:222:LYS:HE2	3:D:1007:HOH:O	2.08	0.53
1:C:254:LYS:HB3	1:C:264:LEU:HD13	1.91	0.53
1:D:305:SER:HA	1:G:48:GLN:HG3	1.91	0.53
1:D:47:ARG:NH2	1:G:220:ASP:O	2.42	0.53
1:C:71:VAL:HG11	1:C:76:VAL:HG11	1.92	0.52
1:A:254:LYS:HB3	1:A:264:LEU:HD13	1.91	0.51
1:D:120:ILE:O	1:D:124:LEU:HG	2.10	0.51
1:H:71:VAL:HG11	1:H:76:VAL:HG11	1.91	0.51
1:A:71:VAL:HG11	1:A:76:VAL:HG11	1.93	0.51
1:B:71:VAL:HG12	1:B:71:VAL:O	2.12	0.50
1:A:4:PHE:CD1	1:A:4:PHE:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1001:DTT:S4	2:A:1001:DTT:C1	2.99	0.49
1:B:47:ARG:NH1	1:B:50:ARG:HA	2.27	0.49
1:H:78:THR:HG22	3:H:1010:HOH:O	2.13	0.48
1:G:4:PHE:N	1:G:4:PHE:CD1	2.81	0.47
1:B:111:LEU:HD22	1:B:115:GLU:HB2	1.97	0.47
1:F:51:ALA:HB3	1:H:218:LEU:HD21	1.96	0.47
1:D:218:LEU:CD2	1:G:51:ALA:HB3	2.45	0.47
1:B:71:VAL:HG11	1:B:76:VAL:HG11	1.97	0.46
1:B:8:LYS:HB2	1:B:11:ASP:OD2	2.16	0.46
1:A:147:LEU:HG	1:A:155:PRO:HB2	1.98	0.45
1:C:4:PHE:N	1:C:4:PHE:CD1	2.84	0.45
1:G:137:HIS:HB3	1:G:140:LEU:HD13	1.98	0.45
1:H:4:PHE:CD1	1:H:4:PHE:N	2.84	0.45
1:H:115:GLU:O	1:H:118:SER:HB2	2.17	0.45
1:D:47:ARG:NH1	1:D:50:ARG:HA	2.32	0.45
1:A:4:PHE:N	1:A:4:PHE:HD1	2.15	0.45
1:B:137:HIS:CG	1:B:140:LEU:HD13	2.52	0.44
1:C:19:LEU:CD1	1:C:29:LYS:HB2	2.47	0.44
1:B:85:ASN:O	1:B:86:ARG:C	2.61	0.44
1:F:4:PHE:CD1	1:F:4:PHE:N	2.85	0.43
1:D:51:ALA:HB2	1:G:218:LEU:CD1	2.47	0.43
1:F:115:GLU:O	1:F:118:SER:HB2	2.19	0.43
1:C:53:ARG:HA	3:C:1028:HOH:O	2.18	0.43
1:F:71:VAL:CG1	1:F:76:VAL:HG11	2.44	0.43
1:H:137:HIS:HB3	1:H:140:LEU:HD13	2.01	0.43
1:A:19:LEU:CD1	1:A:29:LYS:HB2	2.49	0.43
1:A:120:ILE:O	1:A:124:LEU:HG	2.19	0.43
1:F:47:ARG:HB3	1:F:47:ARG:HH11	1.84	0.43
1:C:147:LEU:HG	1:C:155:PRO:HB2	2.00	0.43
1:D:71:VAL:HG11	1:D:76:VAL:HG11	2.00	0.43
1:G:4:PHE:N	1:G:4:PHE:HD1	2.16	0.42
1:B:53:ARG:HD2	3:B:1028:HOH:O	2.20	0.42
1:G:71:VAL:HG11	1:G:76:VAL:HG11	2.00	0.42
1:C:136:ALA:HB2	1:C:196:LEU:HD23	2.01	0.42
1:E:4:PHE:CD1	1:E:4:PHE:N	2.88	0.42
1:G:111:LEU:HD22	1:G:115:GLU:HB2	2.02	0.42
1:A:71:VAL:O	1:A:71:VAL:HG12	2.19	0.41
1:B:137:HIS:HB3	1:B:140:LEU:HD13	2.02	0.41
1:D:4:PHE:CD1	1:D:4:PHE:N	2.85	0.41
1:A:212:SER:HB3	1:A:241:PHE:CZ	2.55	0.41
1:D:71:VAL:HG12	1:D:71:VAL:O	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:HIS:HB3	1:A:140:LEU:HD13	2.01	0.41
1:B:147:LEU:HG	1:B:155:PRO:HB2	2.02	0.41
1:H:4:PHE:N	1:H:4:PHE:HD1	2.18	0.41
1:A:111:LEU:HD12	1:A:291:VAL:HG21	2.03	0.41
1:C:47:ARG:HH11	1:C:47:ARG:HB3	1.84	0.41
2:G:1006:DTT:S4	2:G:1006:DTT:S1	3.15	0.41
1:F:147:LEU:HG	1:F:155:PRO:HB2	2.03	0.41
1:A:31:ARG:NH1	1:A:36:GLY:O	2.53	0.41
1:E:136:ALA:O	1:E:165:ALA:HA	2.21	0.41
1:G:47:ARG:HH11	1:G:47:ARG:HB3	1.86	0.41
1:E:111:LEU:HD22	1:E:115:GLU:HB2	2.03	0.40
1:E:137:HIS:HB3	1:E:140:LEU:HD13	2.02	0.40
1:C:120:ILE:O	1:C:124:LEU:HG	2.21	0.40
1:D:2:GLU:OE2	1:D:2:GLU:HA	2.21	0.40
1:D:218:LEU:CD1	1:G:51:ALA:HB2	2.51	0.40
1:B:86:ARG:HD2	3:B:1013:HOH:O	2.22	0.40
1:C:70:GLN:NE2	1:C:167:GLU:OE1	2.52	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	302/321 (94%)	287 (95%)	13 (4%)	2 (1%)	18	53
1	B	301/321 (94%)	287 (95%)	13 (4%)	1 (0%)	36	70
1	C	301/321 (94%)	287 (95%)	12 (4%)	2 (1%)	18	53
1	D	302/321 (94%)	288 (95%)	13 (4%)	1 (0%)	36	70
1	E	301/321 (94%)	289 (96%)	12 (4%)	0	100	100
1	F	301/321 (94%)	291 (97%)	10 (3%)	0	100	100
1	G	301/321 (94%)	293 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	302/321 (94%)	290 (96%)	11 (4%)	1 (0%)	36	70
All	All	2411/2568 (94%)	2312 (96%)	92 (4%)	7 (0%)	36	70

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	PHE
1	A	161	ASP
1	C	161	ASP
1	A	20	GLY
1	C	20	GLY
1	H	20	GLY
1	D	20	GLY

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	272/288 (94%)	259 (95%)	13 (5%)	23	57
1	B	271/288 (94%)	257 (95%)	14 (5%)	21	55
1	C	271/288 (94%)	259 (96%)	12 (4%)	25	60
1	D	272/288 (94%)	260 (96%)	12 (4%)	25	60
1	E	271/288 (94%)	259 (96%)	12 (4%)	25	60
1	F	271/288 (94%)	257 (95%)	14 (5%)	21	55
1	G	271/288 (94%)	257 (95%)	14 (5%)	21	55
1	H	271/288 (94%)	258 (95%)	13 (5%)	23	57
All	All	2170/2304 (94%)	2066 (95%)	104 (5%)	23	57

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN

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Mol	Chain	Res	Type
1	A	19	LEU
1	A	47	ARG
1	A	53	ARG
1	A	68	LEU
1	A	107	GLN
1	A	111	LEU
1	A	118	SER
1	A	140	LEU
1	A	147	LEU
1	A	262	LYS
1	A	264	LEU
1	A	281	GLN
1	B	19	LEU
1	B	47	ARG
1	B	53	ARG
1	B	68	LEU
1	B	71	VAL
1	B	107	GLN
1	B	111	LEU
1	B	118	SER
1	B	140	LEU
1	B	147	LEU
1	B	262	LYS
1	B	264	LEU
1	B	290	VAL
1	B	294	GLU
1	C	6	GLN
1	C	19	LEU
1	C	47	ARG
1	C	53	ARG
1	C	68	LEU
1	C	111	LEU
1	C	118	SER
1	C	140	LEU
1	C	147	LEU
1	C	262	LYS
1	C	290	VAL
1	C	294	GLU
1	D	6	GLN
1	D	19	LEU
1	D	47	ARG
1	D	53	ARG

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Mol	Chain	Res	Type
1	D	68	LEU
1	D	107	GLN
1	D	111	LEU
1	D	140	LEU
1	D	147	LEU
1	D	262	LYS
1	D	281	GLN
1	D	290	VAL
1	E	6	GLN
1	E	19	LEU
1	E	47	ARG
1	E	53	ARG
1	E	68	LEU
1	E	107	GLN
1	E	111	LEU
1	E	118	SER
1	E	140	LEU
1	E	147	LEU
1	E	262	LYS
1	E	290	VAL
1	F	6	GLN
1	F	19	LEU
1	F	47	ARG
1	F	53	ARG
1	F	68	LEU
1	F	107	GLN
1	F	111	LEU
1	F	140	LEU
1	F	147	LEU
1	F	221	THR
1	F	262	LYS
1	F	281	GLN
1	F	290	VAL
1	F	294	GLU
1	G	6	GLN
1	G	19	LEU
1	G	47	ARG
1	G	53	ARG
1	G	68	LEU
1	G	107	GLN
1	G	111	LEU
1	G	118	SER

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Mol	Chain	Res	Type
1	G	140	LEU
1	G	147	LEU
1	G	221	THR
1	G	262	LYS
1	G	290	VAL
1	G	294	GLU
1	H	6	GLN
1	H	19	LEU
1	H	47	ARG
1	H	53	ARG
1	H	68	LEU
1	H	107	GLN
1	H	111	LEU
1	H	140	LEU
1	H	147	LEU
1	H	262	LYS
1	H	281	GLN
1	H	290	VAL
1	H	294	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	166	HIS
1	A	223	GLN
1	B	75	ASN
1	B	144	ASN
1	B	166	HIS
1	B	223	GLN
1	B	267	GLN
1	C	6	GLN
1	C	85	ASN
1	C	144	ASN
1	C	223	GLN
1	C	267	GLN
1	D	23	GLN
1	D	70	GLN
1	D	128	ASN
1	D	144	ASN
1	D	166	HIS
1	D	223	GLN

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Mol	Chain	Res	Type
1	E	6	GLN
1	E	23	GLN
1	E	70	GLN
1	E	75	ASN
1	E	80	HIS
1	E	85	ASN
1	E	128	ASN
1	E	144	ASN
1	E	223	GLN
1	E	295	ASN
1	F	23	GLN
1	F	75	ASN
1	F	85	ASN
1	F	128	ASN
1	F	144	ASN
1	F	166	HIS
1	F	223	GLN
1	G	6	GLN
1	G	23	GLN
1	G	70	GLN
1	G	75	ASN
1	G	85	ASN
1	G	144	ASN
1	G	223	GLN
1	G	267	GLN
1	H	6	GLN
1	H	23	GLN
1	H	48	GLN
1	H	75	ASN
1	H	80	HIS
1	H	85	ASN
1	H	128	ASN
1	H	144	ASN
1	H	223	GLN
1	H	295	ASN

5.3.3 RNA ⓘ

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](#)

8 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	DTT	E	1005	-	7,7,7	0.53	0	4,8,8	1.18	0
2	DTT	G	1006	-	7,7,7	0.57	0	4,8,8	0.54	0
2	DTT	B	1002	-	7,7,7	0.67	0	4,8,8	0.70	0
2	DTT	F	1007	-	7,7,7	0.60	0	4,8,8	0.52	0
2	DTT	H	1008	-	7,7,7	0.57	0	4,8,8	0.49	0
2	DTT	A	1001	-	7,7,7	0.57	0	4,8,8	0.86	0
2	DTT	D	1004	-	7,7,7	0.74	0	4,8,8	0.89	0
2	DTT	C	1003	-	7,7,7	0.59	0	4,8,8	0.80	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
2	DTT	E	1005	-	1/1/2/2	4/8/8/8	-
2	DTT	G	1006	-	1/1/2/2	3/8/8/8	-
2	DTT	B	1002	-	1/1/2/2	4/8/8/8	-
2	DTT	F	1007	-	1/1/2/2	4/8/8/8	-
2	DTT	H	1008	-	1/1/2/2	3/8/8/8	-
2	DTT	A	1001	-	1/1/2/2	3/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTT	D	1004	-	1/1/2/2	6/8/8/8	-
2	DTT	C	1003	-	1/1/2/2	4/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	DTT	C3
2	B	1002	DTT	C3
2	C	1003	DTT	C3
2	D	1004	DTT	C3
2	E	1005	DTT	C3
2	F	1007	DTT	C3
2	G	1006	DTT	C3
2	H	1008	DTT	C3

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	DTT	C1-C2-C3-C4
2	B	1002	DTT	C1-C2-C3-O3
2	B	1002	DTT	C1-C2-C3-C4
2	B	1002	DTT	O2-C2-C3-O3
2	B	1002	DTT	O2-C2-C3-C4
2	C	1003	DTT	S1-C1-C2-C3
2	C	1003	DTT	C1-C2-C3-C4
2	D	1004	DTT	C1-C2-C3-O3
2	D	1004	DTT	C1-C2-C3-C4
2	D	1004	DTT	O2-C2-C3-O3
2	D	1004	DTT	O2-C2-C3-C4
2	D	1004	DTT	C2-C3-C4-S4
2	D	1004	DTT	O3-C3-C4-S4
2	E	1005	DTT	C1-C2-C3-C4
2	F	1007	DTT	S1-C1-C2-C3
2	F	1007	DTT	C2-C3-C4-S4
2	F	1007	DTT	O3-C3-C4-S4
2	G	1006	DTT	S1-C1-C2-C3
2	G	1006	DTT	C2-C3-C4-S4
2	G	1006	DTT	O3-C3-C4-S4
2	H	1008	DTT	S1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	H	1008	DTT	C2-C3-C4-S4
2	H	1008	DTT	O3-C3-C4-S4
2	A	1001	DTT	C1-C2-C3-O3
2	E	1005	DTT	C1-C2-C3-O3
2	C	1003	DTT	O3-C3-C4-S4
2	E	1005	DTT	O3-C3-C4-S4
2	C	1003	DTT	C1-C2-C3-O3
2	E	1005	DTT	C2-C3-C4-S4
2	A	1001	DTT	O2-C2-C3-O3
2	F	1007	DTT	C1-C2-C3-C4

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1005	DTT	1	0
2	G	1006	DTT	1	0
2	F	1007	DTT	1	0
2	H	1008	DTT	2	0
2	A	1001	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 ⓘ

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	304/321 (94%)	0.53	7 (2%) 61 38	94, 99, 104, 121	0
1	B	303/321 (94%)	0.39	6 (1%) 65 41	94, 99, 104, 113	0
1	C	303/321 (94%)	0.46	7 (2%) 61 38	94, 99, 103, 111	0
1	D	304/321 (94%)	0.34	5 (1%) 70 47	95, 99, 103, 112	0
1	E	303/321 (94%)	0.51	10 (3%) 49 28	94, 99, 103, 109	0
1	F	303/321 (94%)	0.21	3 (0%) 79 59	96, 99, 103, 106	0
1	G	303/321 (94%)	0.08	1 (0%) 90 79	95, 99, 103, 106	0
1	H	304/321 (94%)	-0.02	1 (0%) 90 79	95, 99, 103, 111	0
All	All	2427/2568 (94%)	0.31	40 (1%) 70 47	94, 99, 103, 121	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	51	ALA	3.3
1	H	305	SER	3.2
1	C	49	SER	3.0
1	E	51	ALA	3.0
1	D	281	GLN	3.0
1	A	278	VAL	2.9
1	F	48	GLN	2.9
1	F	300	TYR	2.8
1	B	22	GLY	2.8
1	B	49	SER	2.7
1	A	302	ARG	2.7
1	E	304	ARG	2.6
1	A	300	TYR	2.5
1	E	176	ASN	2.5
1	D	53	ARG	2.5
1	E	191	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	48	GLN	2.5
1	E	35	THR	2.4
1	E	49	SER	2.4
1	C	302	ARG	2.4
1	C	191	TYR	2.4
1	G	49	SER	2.4
1	A	283	ALA	2.4
1	F	24	PHE	2.3
1	E	193	PRO	2.3
1	B	52	SER	2.3
1	E	291	VAL	2.3
1	E	290	VAL	2.3
1	C	189	VAL	2.2
1	E	288	GLU	2.2
1	B	51	ALA	2.1
1	D	284	MET	2.1
1	C	186	PRO	2.1
1	A	143	GLU	2.1
1	C	258	LYS	2.1
1	B	302	ARG	2.1
1	A	51	ALA	2.1
1	C	218	LEU	2.0
1	B	300	TYR	2.0
1	D	285	VAL	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
2	DTT	G	1006	8/8	0.63	0.17	134,136,137,139	0
2	DTT	H	1008	8/8	0.72	0.16	136,137,138,140	0
2	DTT	F	1007	8/8	0.85	0.19	123,124,125,125	0
2	DTT	D	1004	8/8	0.87	0.20	114,117,118,119	0
2	DTT	E	1005	8/8	0.89	0.23	102,103,104,104	0
2	DTT	C	1003	8/8	0.92	0.24	74,79,81,81	0
2	DTT	A	1001	8/8	0.93	0.20	93,96,97,98	0
2	DTT	B	1002	8/8	0.95	0.23	72,73,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.