



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:04 AM UTC

PDB ID : 3RTY / pdb_00003rty
Title : Structure of an Enclosed Dimer Formed by The Drosophila Period Protein
Authors : King, H.A.; Hoelz, A.; Crane, B.R.; Young, M.W.
Deposited on : 2011-05-04
Resolution : 2.85 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

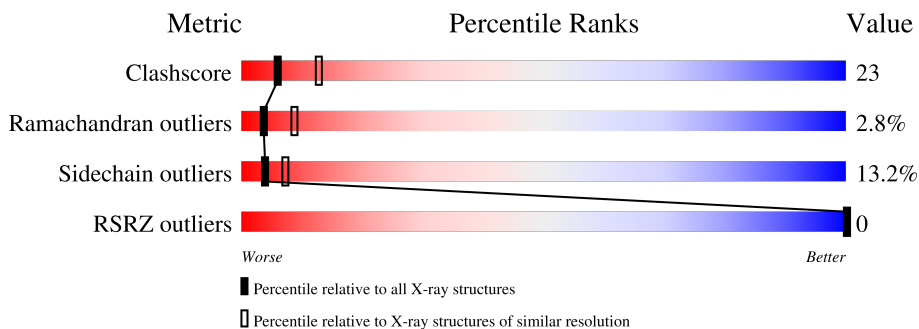
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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))
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	339	
1	B	339	
1	C	339	
1	D	339	
1	E	339	
1	F	339	
1	G	339	

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Mol	Chain	Length	Quality of chain
1	H	339	 47% 32% 10% 11%

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	C	903	-	-	X	-
2	DTT	F	900	-	-	X	-
2	DTT	F	903	-	-	X	-
2	DTT	H	903	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19848 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.

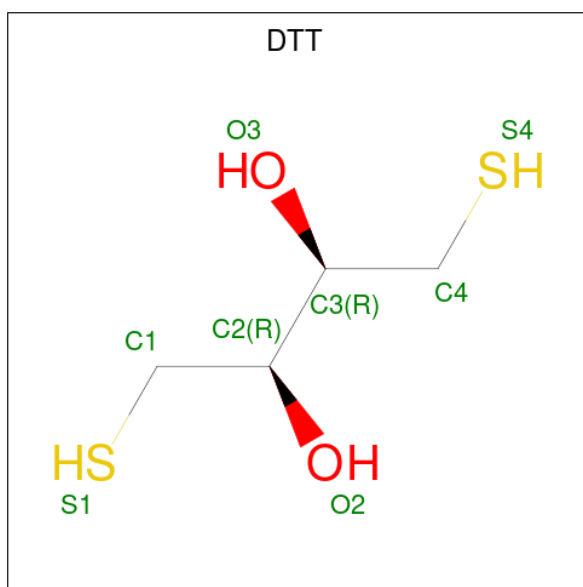
- Molecule 1 is a protein called Period circadian protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	306	2436	1549	419	450	18	0	0	0
1	B	302	2410	1530	415	447	18	0	0	0
1	C	302	2410	1530	415	447	18	0	0	0
1	D	306	2436	1549	419	450	18	0	0	0
1	E	307	2443	1554	420	451	18	0	0	0
1	F	302	2410	1530	415	447	18	0	0	0
1	G	306	2436	1549	419	450	18	0	0	0
1	H	302	2410	1530	415	447	18	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	543	GLU	ASP	conflict	UNP P07663
B	543	GLU	ASP	conflict	UNP P07663
C	543	GLU	ASP	conflict	UNP P07663
D	543	GLU	ASP	conflict	UNP P07663
E	543	GLU	ASP	conflict	UNP P07663
F	543	GLU	ASP	conflict	UNP P07663
G	543	GLU	ASP	conflict	UNP P07663
H	543	GLU	ASP	conflict	UNP P07663

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



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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total 34	O 34	0	0
3	B	31	Total 31	O 31	0	0
3	C	26	Total 26	O 26	0	0
3	D	28	Total 28	O 28	0	0
3	E	32	Total 32	O 32	0	0

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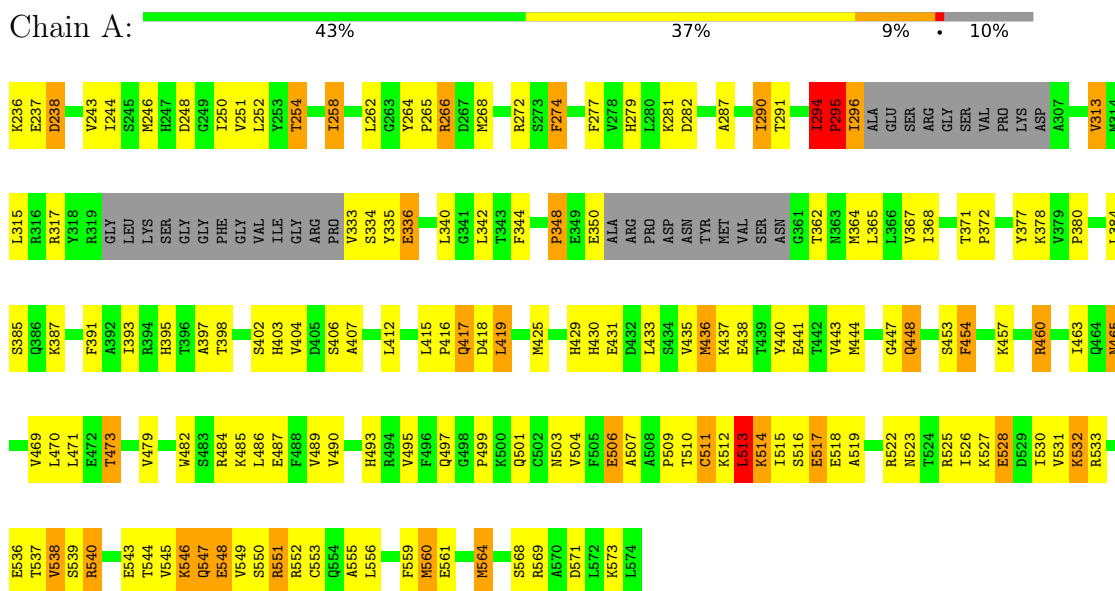
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	33	Total 33	O 33	0	0
3	G	28	Total 28	O 28	0	0
3	H	21	Total 21	O 21	0	0

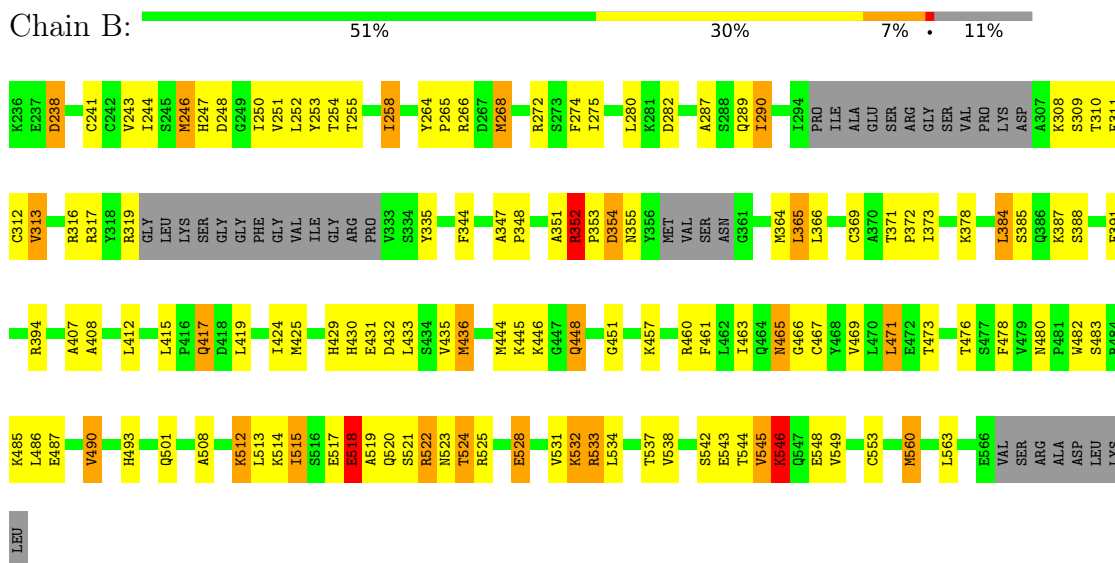
3 Residue-property plots

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: Period circadian protein



- Molecule 1: Period circadian protein



K236	V313	P380	C467	V549
E237	R316	D881	Y468	S550
D238	R317	E382	V469	R551
S239	I383	I383	L470	R552
F240	Y318	L384	L471	C553
M246	R319	K387	T476	L556
H247	GLY	N480	M480	A557
D248	LEU	F391	N480	M560
G249	LYS	H395	S483	E561
I250	SER	T396	R484	T562
V251	GLY	A397	K485	E586
L252	PHE	F398	L486	VAL
Y253	GLY	G399	V490	SER
T254	VAL	I400	R494	ARG
S257	ILE	I401	V495	ALA
I258	GLY	V404	F496	ASP
ARG	ARG	D405	Q497	LEU
T259	PRO	A407	Q501	LYS
T260	PRO	S410	V504	LEU
D260	Y383	A411	A507	T510
V261	S394	L412	C511	K512
L262	S394	L342	L513	K514
G263	Y335	T343	K514	L515
Y264	L340	F344	S116	E517
P265	G341	L415	E518	E518
R266	L342	P416	A519	A519
D267	L342	Q417	Q520	R522
M268	T343	D418	S521	N523
R272	F344	L419	R522	T524
L280	A347	I424	M436	R525
R281	P348	M425	E528	E528
D282	E349	H429	V531	K532
A287	E350	H430	R533	R533
S288	A351	E431	L534	L534
Q289	R352	D432	T537	T537
L290	P353	M436	V538	V538
T291	D354	T442	T544	T544
I294	M355	V443	V545	V545
PRO	Y386	M444	R546	Q547
ILE	VAL	K445	E548	E548
ALA	VAL	K446		
GLU	ASN	G447		
SER	G361	Q448		
ARG	M364	K457		
GLY	L365	P458		
LYS	L366	Y459		
GLY	L367	R460		
SER	V367	I463		
VAL	I368	Q464		
PRO	C369	M465		
ASP	A370	N465		
ASP	T371	Q464		
A307	P372	R460		
K308	I373	I463		
S309	S376	Q464		
T310	Y377	M465		
F311	K378	G466		
C312	V379			

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.41Å 94.70Å 141.03Å 88.19° 89.63° 89.87°	Depositor
Resolution (Å)	20.01 – 2.85 20.01 – 2.85	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.01-2.85) 87.0 (20.01-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.83Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.239 , 0.289 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.096 for h,-k,-l 0.075 for -h,k,-l 0.075 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19848	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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

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	1/2486 (0.0%)	1.12	19/3355 (0.6%)
1	B	0.61	0/2461	1.08	9/3322 (0.3%)
1	C	0.59	0/2461	1.08	11/3322 (0.3%)
1	D	0.62	1/2486 (0.0%)	1.13	21/3355 (0.6%)
1	E	0.64	1/2494 (0.0%)	1.17	23/3366 (0.7%)
1	F	0.62	0/2461	1.08	16/3322 (0.5%)
1	G	0.63	1/2486 (0.0%)	1.17	26/3355 (0.8%)
1	H	0.56	0/2461	1.07	11/3322 (0.3%)
All	All	0.61	4/19796 (0.0%)	1.11	136/26719 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	512	LYS	CA-C	6.58	1.61	1.52
1	E	333	VAL	CA-CB	6.40	1.61	1.53
1	D	379	VAL	CA-CB	5.23	1.60	1.54
1	A	385	SER	CA-C	5.08	1.54	1.52

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	ASN	N-CA-C	10.29	125.33	108.96
1	F	355	ASN	N-CA-C	10.25	124.93	109.25
1	B	354	ASP	N-CA-C	9.79	124.64	108.48
1	C	355	ASN	N-CA-C	9.72	124.12	109.25
1	D	386	GLN	N-CA-C	-9.71	101.43	113.18

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	2436	0	2441	131	0
1	B	2410	0	2396	108	0
1	C	2410	0	2396	116	0
1	D	2436	0	2442	124	0
1	E	2443	0	2447	125	0
1	F	2410	0	2392	109	0
1	G	2436	0	2438	92	0
1	H	2410	0	2392	117	0
2	A	32	0	36	3	0
2	B	32	0	35	3	0
2	C	32	0	36	7	0
2	D	24	0	27	2	0
2	E	16	0	18	0	0
2	F	32	0	36	8	0
2	G	24	0	27	2	0
2	H	32	0	36	5	0
3	A	34	0	0	0	0
3	B	31	0	0	0	0
3	C	26	0	0	0	0
3	D	28	0	0	0	0
3	E	32	0	0	0	0
3	F	33	0	0	0	0
3	G	28	0	0	0	0
3	H	21	0	0	1	0
All	All	19848	0	19595	890	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 23.

The worst 5 of 890 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:C:521:SER:HB3	1:C:525:ARG:HH12	1.24	1.03
1:G:457:LYS:H	1:G:457:LYS:HD3	1.23	1.02
1:H:457:LYS:H	1:H:457:LYS:HD3	1.24	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:LYS:H	1:C:457:LYS:HD3	1.20	1.00
1:F:501:GLN:HE21	1:F:508:ALA:HB1	1.23	1.00

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	298/339 (88%)	265 (89%)	23 (8%)	10 (3%)	3 6
1	B	294/339 (87%)	261 (89%)	25 (8%)	8 (3%)	4 9
1	C	294/339 (87%)	264 (90%)	24 (8%)	6 (2%)	6 13
1	D	298/339 (88%)	269 (90%)	19 (6%)	10 (3%)	3 6
1	E	299/339 (88%)	267 (89%)	21 (7%)	11 (4%)	2 5
1	F	294/339 (87%)	262 (89%)	25 (8%)	7 (2%)	4 10
1	G	298/339 (88%)	266 (89%)	23 (8%)	9 (3%)	3 8
1	H	294/339 (87%)	259 (88%)	29 (10%)	6 (2%)	6 13
All	All	2369/2712 (87%)	2113 (89%)	189 (8%)	67 (3%)	4 9

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ARG
1	A	513	LEU
1	A	516	SER
1	A	517	GLU
1	B	266	ARG

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	273/298 (92%)	238 (87%)	35 (13%)	4	7
1	B	269/298 (90%)	233 (87%)	36 (13%)	4	7
1	C	269/298 (90%)	229 (85%)	40 (15%)	3	5
1	D	273/298 (92%)	236 (86%)	37 (14%)	3	7
1	E	274/298 (92%)	245 (89%)	29 (11%)	6	13
1	F	269/298 (90%)	233 (87%)	36 (13%)	4	7
1	G	273/298 (92%)	243 (89%)	30 (11%)	6	12
1	H	269/298 (90%)	225 (84%)	44 (16%)	2	4
All	All	2169/2384 (91%)	1882 (87%)	287 (13%)	4	7

5 of 287 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	460	ARG
1	H	562	THR
1	G	528	GLU
1	H	404	VAL
1	C	471	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	493	HIS
1	H	417	GLN
1	F	547	GLN
1	G	465	ASN
1	H	492	HIS

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](#)

28 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	G	902	1	7,7,7	0.94	0	4,8,8	0.27	0
2	DTT	D	902	1	7,7,7	0.97	0	4,8,8	0.41	0
2	DTT	C	902	1	7,7,7	0.93	0	4,8,8	0.48	0
2	DTT	H	901	1	7,7,7	0.96	0	4,8,8	0.71	0
2	DTT	F	901	1	7,7,7	0.90	0	4,8,8	0.50	0
2	DTT	C	901	1	7,7,7	0.83	0	4,8,8	0.19	0
2	DTT	A	901	1	7,7,7	1.05	0	4,8,8	0.67	0
2	DTT	H	903	1	7,7,7	1.11	1 (14%)	4,8,8	0.61	0
2	DTT	F	900	1	7,7,7	0.84	0	4,8,8	0.51	0
2	DTT	E	900	1	7,7,7	0.76	0	4,8,8	0.37	0
2	DTT	F	903	1	7,7,7	1.45	1 (14%)	4,8,8	0.52	0
2	DTT	B	900	1	7,7,7	0.82	0	4,8,8	0.66	0
2	DTT	G	901	1	7,7,7	1.05	0	4,8,8	0.63	0
2	DTT	C	903	1	7,7,7	1.35	1 (14%)	4,8,8	0.77	0
2	DTT	A	902	1	7,7,7	0.89	0	4,8,8	0.46	0
2	DTT	H	900	1	7,7,7	0.82	0	4,8,8	0.47	0
2	DTT	B	903	1	7,7,7	0.96	0	4,8,8	0.20	0
2	DTT	D	901	1	7,7,7	1.01	0	4,8,8	0.58	0
2	DTT	D	900	1	7,7,7	0.60	0	4,8,8	0.34	0
2	DTT	C	900	1	7,7,7	0.82	0	4,8,8	0.32	0
2	DTT	A	900	1	7,7,7	0.74	0	4,8,8	0.44	0
2	DTT	B	902	1	7,7,7	0.94	0	4,8,8	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DTT	H	902	1	7,7,7	1.02	0	4,8,8	0.76	0
2	DTT	A	903	1	7,7,7	0.74	0	4,8,8	0.40	0
2	DTT	G	900	1	7,7,7	0.72	0	4,8,8	0.49	0
2	DTT	E	901	1	7,7,7	1.09	1 (14%)	4,8,8	0.72	0
2	DTT	F	902	1	7,7,7	0.77	0	4,8,8	0.45	0
2	DTT	B	901	1	7,7,7	0.90	0	4,8,8	0.63	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	G	902	1	-	3/8/8/8	-
2	DTT	D	902	1	-	5/8/8/8	-
2	DTT	C	902	1	-	6/8/8/8	-
2	DTT	H	901	1	-	5/8/8/8	-
2	DTT	F	901	1	-	5/8/8/8	-
2	DTT	C	901	1	-	6/8/8/8	-
2	DTT	A	901	1	-	7/8/8/8	-
2	DTT	H	903	1	-	2/8/8/8	-
2	DTT	F	900	1	-	5/8/8/8	-
2	DTT	E	900	1	-	2/8/8/8	-
2	DTT	F	903	1	-	2/8/8/8	-
2	DTT	B	900	1	-	6/8/8/8	-
2	DTT	G	901	1	-	7/8/8/8	-
2	DTT	C	903	1	-	6/8/8/8	-
2	DTT	A	902	1	-	3/8/8/8	-
2	DTT	H	900	1	-	6/8/8/8	-
2	DTT	B	903	1	-	1/8/8/8	-
2	DTT	D	901	1	-	6/8/8/8	-
2	DTT	D	900	1	-	4/8/8/8	-
2	DTT	C	900	1	-	6/8/8/8	-
2	DTT	A	900	1	-	5/8/8/8	-
2	DTT	B	902	1	-	4/8/8/8	-
2	DTT	H	902	1	-	4/8/8/8	-
2	DTT	A	903	1	-	4/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTT	G	900	1	-	3/8/8/8	-
2	DTT	E	901	1	-	6/8/8/8	-
2	DTT	F	902	1	-	6/8/8/8	-
2	DTT	B	901	1	-	6/8/8/8	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	903	DTT	C4-S4	3.09	1.87	1.81
2	C	903	DTT	C1-C2	2.58	1.58	1.51
2	H	903	DTT	C3-C2	2.22	1.58	1.53
2	E	901	DTT	C3-C2	2.09	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	DTT	S1-C1-C2-O2
2	A	900	DTT	C1-C2-C3-C4
2	A	900	DTT	O2-C2-C3-C4
2	A	901	DTT	S1-C1-C2-O2
2	A	901	DTT	C1-C2-C3-O3

There are no ring outliers.

16 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	902	DTT	2	0
2	D	902	DTT	1	0
2	H	901	DTT	1	0
2	C	901	DTT	1	0
2	H	903	DTT	4	0
2	F	900	DTT	4	0
2	F	903	DTT	4	0
2	B	900	DTT	1	0
2	C	903	DTT	4	0
2	A	902	DTT	1	0
2	B	903	DTT	1	0
2	D	900	DTT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	900	DTT	2	0
2	A	900	DTT	1	0
2	A	903	DTT	1	0
2	B	901	DTT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	306/339 (90%)	-1.60	0 100 100	31, 56, 125, 134	0
1	B	302/339 (89%)	-1.65	0 100 100	32, 58, 115, 130	0
1	C	302/339 (89%)	-1.58	0 100 100	29, 60, 126, 142	0
1	D	306/339 (90%)	-1.56	0 100 100	31, 63, 130, 147	0
1	E	307/339 (90%)	-1.59	0 100 100	28, 56, 128, 146	0
1	F	302/339 (89%)	-1.59	0 100 100	32, 64, 127, 139	0
1	G	306/339 (90%)	-1.57	0 100 100	30, 58, 128, 136	0
1	H	302/339 (89%)	-1.52	0 100 100	43, 78, 120, 144	0
All	All	2433/2712 (89%)	-1.58	0 100 100	28, 62, 126, 147	0

There are no RSRZ outliers to report.

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
2	DTT	A	903	8/8	0.95	0.07	124,136,139,142	0
2	DTT	B	903	8/8	0.96	0.06	125,135,139,141	0
2	DTT	G	901	8/8	0.96	0.06	103,106,109,110	0
2	DTT	D	902	8/8	0.97	0.07	135,141,142,143	0
2	DTT	D	901	8/8	0.97	0.05	108,115,119,120	0
2	DTT	H	903	8/8	0.97	0.05	135,139,141,142	0
2	DTT	A	901	8/8	0.98	0.04	99,107,111,111	0
2	DTT	A	902	8/8	0.98	0.07	136,140,143,146	0
2	DTT	E	901	8/8	0.98	0.04	104,112,115,116	0
2	DTT	F	900	8/8	0.98	0.04	82,89,95,102	0
2	DTT	F	903	8/8	0.98	0.04	129,136,138,140	0
2	DTT	C	900	8/8	0.98	0.04	77,83,90,99	0
2	DTT	G	902	8/8	0.98	0.07	130,131,132,132	0
2	DTT	H	900	8/8	0.98	0.04	104,105,109,112	0
2	DTT	C	903	8/8	0.98	0.06	125,137,140,143	0
2	DTT	E	900	8/8	0.99	0.03	74,77,82,87	0
2	DTT	B	900	8/8	0.99	0.04	80,83,89,97	0
2	DTT	C	901	8/8	0.99	0.05	96,104,110,114	0
2	DTT	F	901	8/8	0.99	0.05	94,98,103,105	0
2	DTT	F	902	8/8	0.99	0.05	119,120,121,124	0
2	DTT	C	902	8/8	0.99	0.04	102,107,110,115	0
2	DTT	G	900	8/8	0.99	0.03	71,74,85,91	0
2	DTT	B	901	8/8	0.99	0.03	85,90,97,100	0
2	DTT	D	900	8/8	0.99	0.03	71,75,81,88	0
2	DTT	B	902	8/8	0.99	0.05	98,106,112,117	0
2	DTT	H	901	8/8	0.99	0.04	112,117,120,121	0
2	DTT	H	902	8/8	0.99	0.06	96,100,104,110	0
2	DTT	A	900	8/8	0.99	0.04	74,77,84,89	0

6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.