



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 11:21 PM EDT

PDB ID : 3RTY  
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

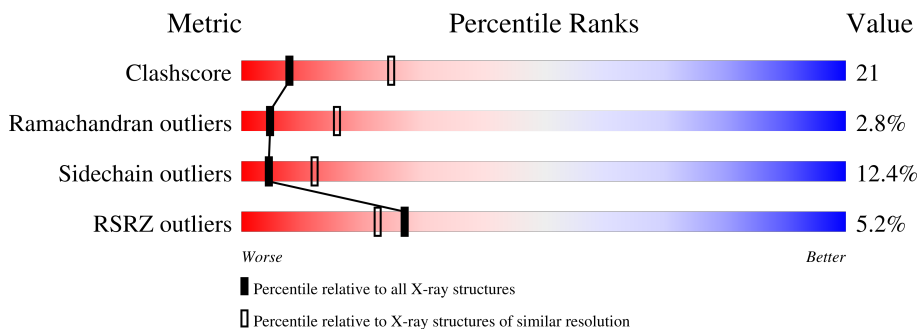
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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  $\geq 3$ , 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	 4% 47% 36% 7% 10%
1	B	339	 3% 53% 30% 6% 11%
1	C	339	 4% 51% 29% 8% 11%
1	D	339	 6% 48% 36% 6% 10%
1	E	339	 7% 47% 36% 7% 9%
1	F	339	 4% 52% 31% 6% 11%
1	G	339	 5% 57% 29% 5% 10%

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Mol	Chain	Length	Quality of chain
1	H	339	

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	902	-	-	-	X
2	DTT	A	903	-	-	-	X
2	DTT	C	903	-	-	X	X
2	DTT	D	901	-	-	-	X
2	DTT	D	902	-	-	-	X
2	DTT	F	900	-	-	X	-
2	DTT	F	903	-	-	X	-
2	DTT	G	901	-	-	-	X
2	DTT	G	902	-	-	-	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.

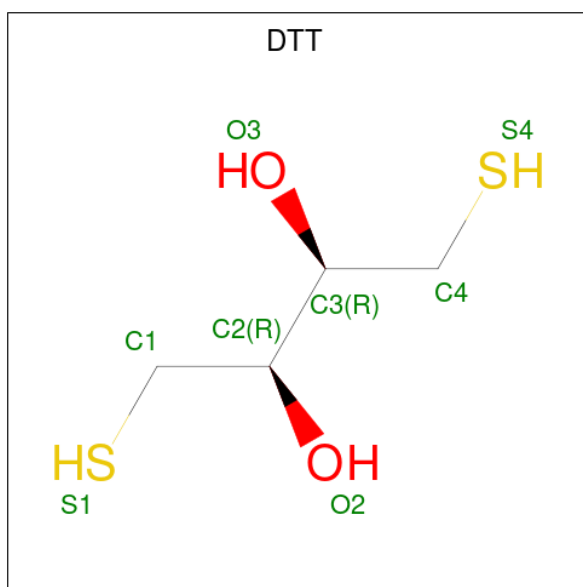
- Molecule 1 is a protein called Period circadian protein.

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 (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



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

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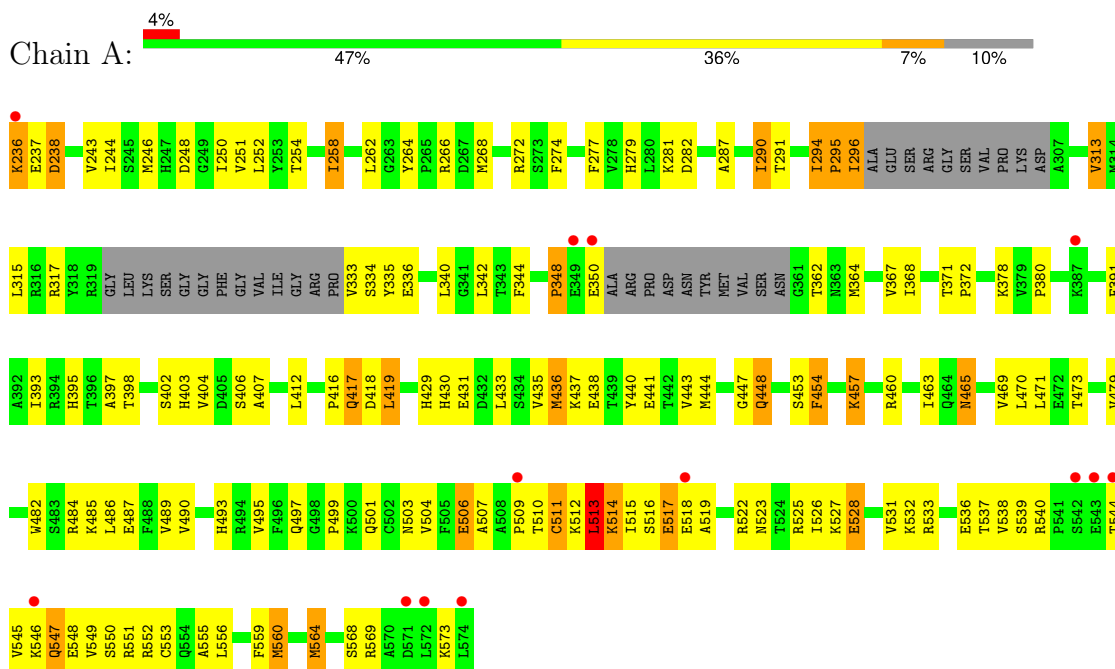
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	F	33	Total 33	O 33	0	0
3	G	28	Total 28	O 28	0	0
3	H	21	Total 21	O 21	0	0

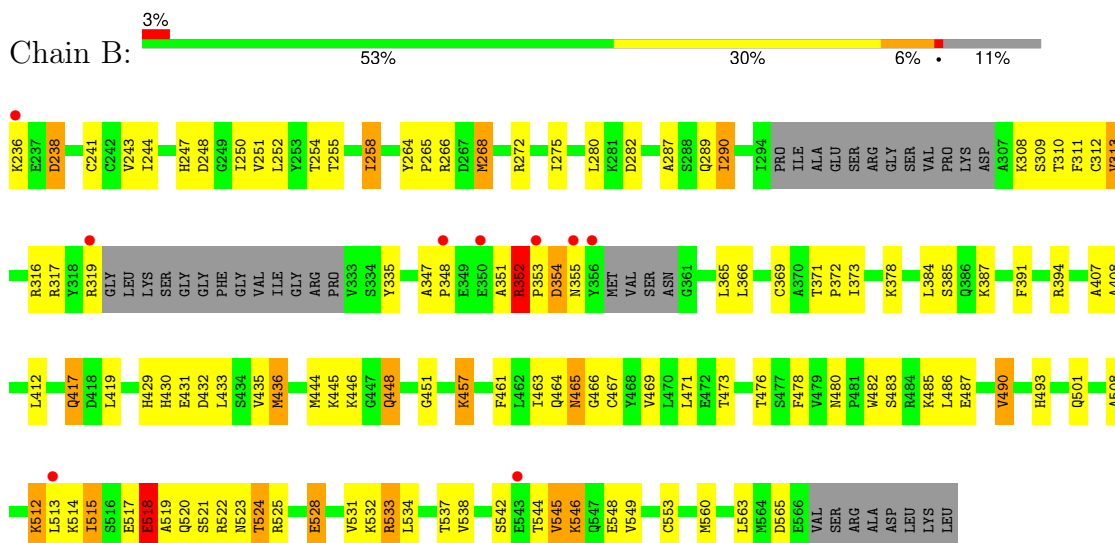
### 3 Residue-property plots i

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: Period circadian protein



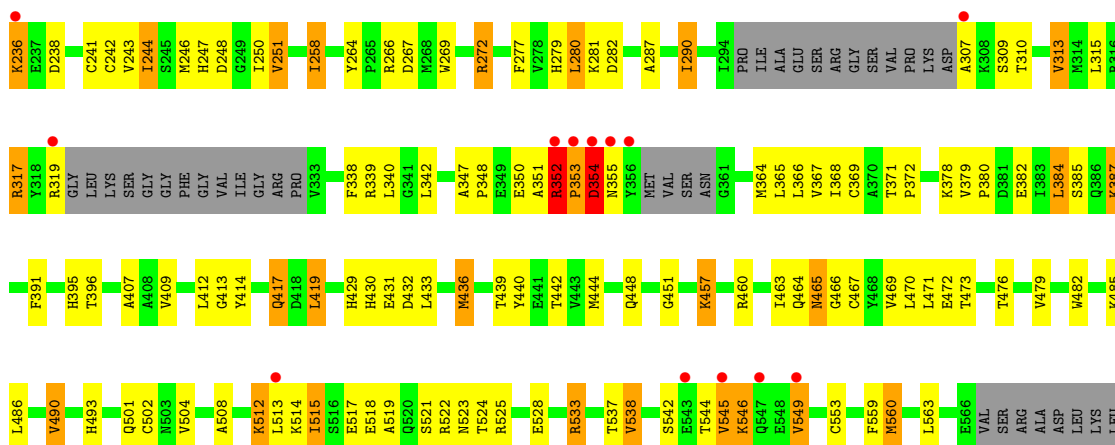
- Molecule 1: Period circadian protein





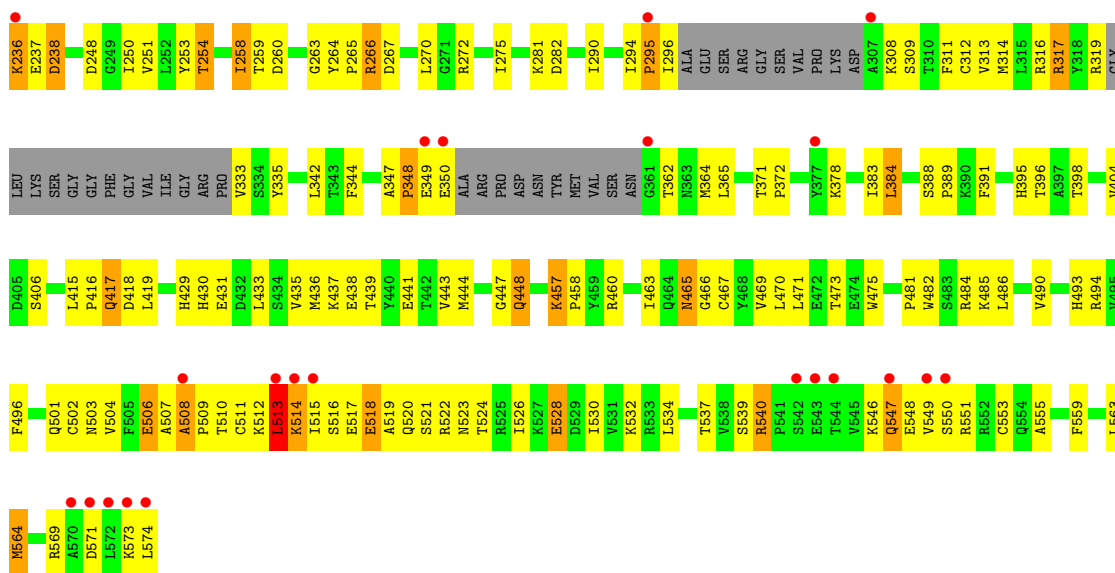
## ● Molecule 1: Period circadian protein

Chain C: 4% 51% 29% 8% 11%



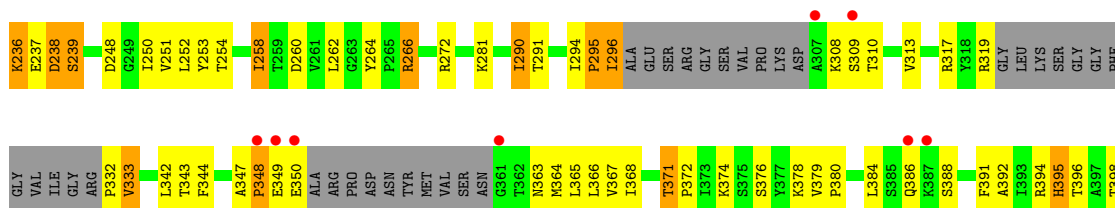
## ● Molecule 1: Period circadian protein

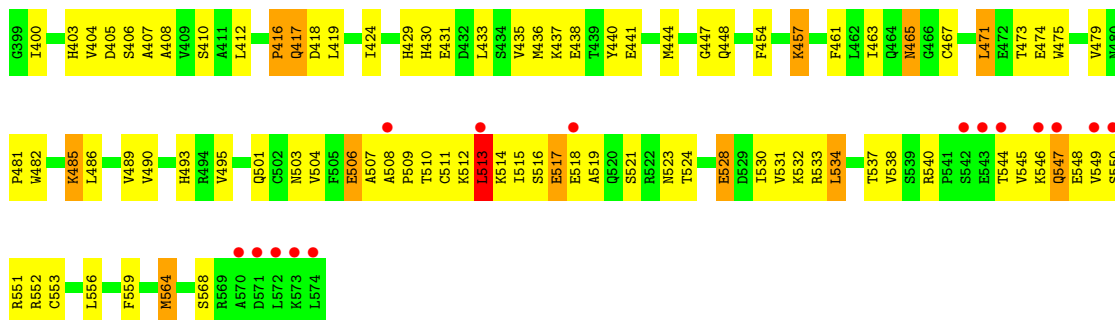
Chain D: 6% 48% 36% 6% 10%



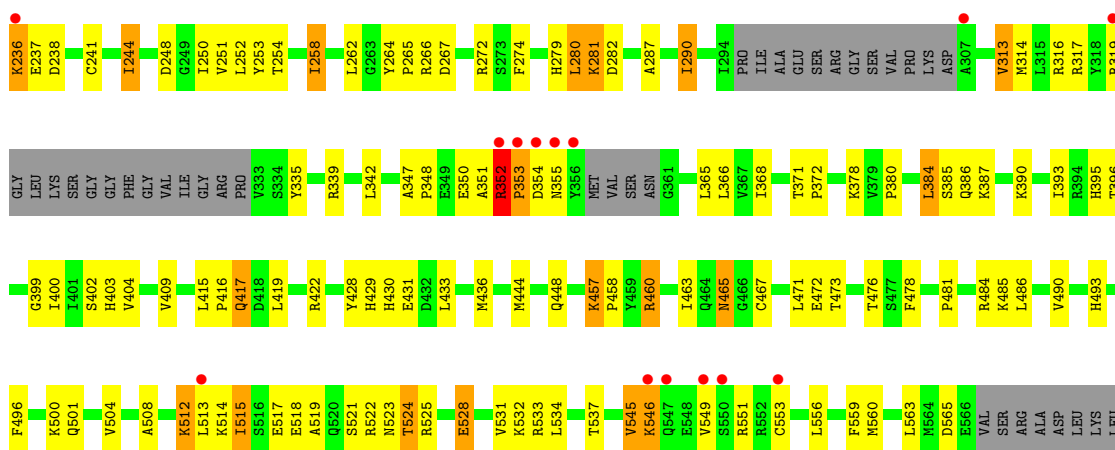
## ● Molecule 1: Period circadian protein

Chain E: 7% 47% 36% 7% 9%

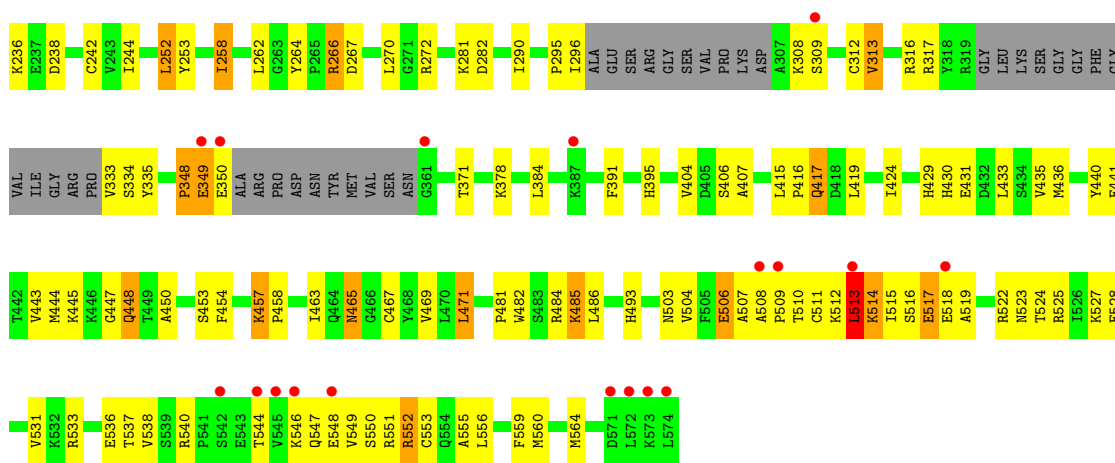




- Molecule 1: Period circadian protein

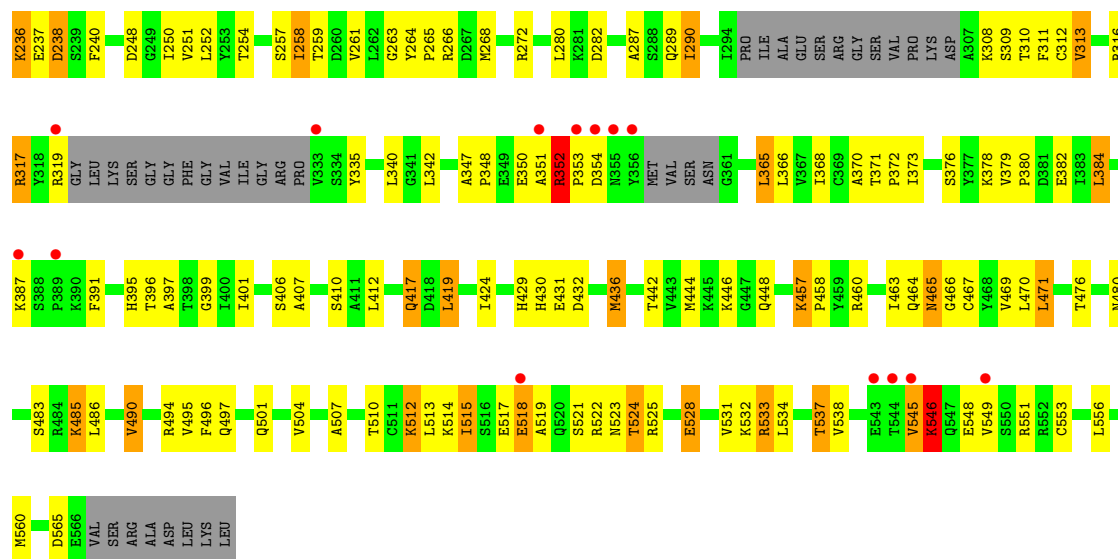


- Molecule 1: Period circadian protein



- Molecule 1: Period circadian protein





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.41Å 94.70Å 141.03Å 88.19° 89.63° 89.87°	Depositor
Resolution (Å)	20.01 – 2.85 20.14 – 2.86	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.01-2.85) 87.0 (20.14-2.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	63.0	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 26.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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	0.89	EDS
Total number of atoms	19848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.47	0/2486	0.74	0/3355
1	B	0.49	0/2461	0.73	2/3322 (0.1%)
1	C	0.48	0/2461	0.71	1/3322 (0.0%)
1	D	0.51	0/2486	0.75	0/3355
1	E	0.51	0/2494	0.76	0/3366
1	F	0.48	0/2461	0.72	1/3322 (0.0%)
1	G	0.50	0/2486	0.75	0/3355
1	H	0.44	0/2461	0.69	0/3322
All	All	0.49	0/19796	0.73	4/26719 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	354	ASP	N-CA-C	5.34	125.43	111.00
1	B	355	ASN	N-CA-C	5.31	125.33	111.00
1	F	355	ASN	N-CA-C	5.16	124.93	111.00
1	B	354	ASP	N-CA-C	5.05	124.64	111.00

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	123	0
1	B	2410	0	2396	97	0
1	C	2410	0	2396	110	0
1	D	2436	0	2442	119	0
1	E	2443	0	2447	116	0
1	F	2410	0	2392	101	0
1	G	2436	0	2438	89	0
1	H	2410	0	2392	108	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	839	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 21.

All (839) 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
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
2:H:903:DTT:S1	2:H:903:DTT:H42	2.02	0.97
1:F:457:LYS:H	1:F:457:LYS:HD3	1.28	0.97
1:C:465:ASN:HD21	1:C:467:CYS:HB2	1.29	0.96
1:D:463:ILE:HD12	1:D:504:VAL:HG23	1.50	0.94
1:C:409:VAL:HG21	2:C:900:DTT:S1	2.08	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:521:SER:HB3	1:F:525:ARG:HH12	1.31	0.92
1:F:500:LYS:O	2:F:903:DTT:S4	2.27	0.92
1:H:317:ARG:HB3	1:H:317:ARG:HH21	1.33	0.92
1:F:380:PRO:HB3	2:F:903:DTT:S4	2.11	0.91
1:B:417:GLN:H	1:B:417:GLN:NE2	1.69	0.90
1:H:465:ASN:ND2	1:H:467:CYS:H	1.71	0.89
1:B:417:GLN:H	1:B:417:GLN:HE21	0.92	0.89
1:E:457:LYS:H	1:E:457:LYS:HD3	1.37	0.88
1:H:417:GLN:H	1:H:417:GLN:HE21	1.22	0.87
1:B:417:GLN:HE21	1:B:417:GLN:N	1.70	0.87
1:C:272:ARG:HG2	1:C:272:ARG:HH11	1.36	0.87
1:D:457:LYS:H	1:D:457:LYS:HD3	1.39	0.87
1:C:417:GLN:H	1:C:417:GLN:HE21	1.23	0.86
1:A:272:ARG:HG2	1:A:272:ARG:HH11	1.40	0.86
1:F:352:ARG:H	1:F:353:PRO:CD	1.89	0.86
1:C:465:ASN:ND2	1:C:467:CYS:H	1.74	0.85
1:A:548:GLU:HA	1:A:551:ARG:HB3	1.58	0.85
1:E:367:VAL:HG21	1:F:563:LEU:HD21	1.58	0.85
1:C:352:ARG:H	1:C:353:PRO:CD	1.90	0.85
1:H:352:ARG:H	1:H:353:PRO:HD2	1.41	0.85
1:F:272:ARG:HG2	1:F:272:ARG:HH11	1.42	0.84
1:H:521:SER:HB3	1:H:525:ARG:HH12	1.42	0.84
1:C:352:ARG:H	1:C:353:PRO:HD2	1.42	0.84
1:G:417:GLN:H	1:G:417:GLN:HE21	1.26	0.84
1:H:347:ALA:HB2	1:H:365:LEU:HD13	1.57	0.84
1:G:548:GLU:HA	1:G:551:ARG:HB3	1.59	0.84
1:D:512:LYS:O	1:D:513:LEU:HB3	1.78	0.83
1:H:391:PHE:HB3	1:H:407:ALA:HB3	1.61	0.83
1:D:258:ILE:HD12	1:D:264:TYR:HB2	1.62	0.81
1:E:404:VAL:HG21	1:E:416:PRO:HA	1.63	0.81
1:G:517:GLU:HG3	1:G:518:GLU:H	1.46	0.80
1:A:457:LYS:H	1:A:457:LYS:HD3	1.45	0.80
1:A:517:GLU:HG3	1:A:518:GLU:H	1.47	0.80
1:B:501:GLN:HE21	1:B:508:ALA:HB1	1.46	0.80
1:E:395:HIS:HE1	1:E:440:TYR:OH	1.65	0.79
1:E:517:GLU:HG3	1:E:518:GLU:H	1.47	0.79
1:E:258:ILE:HD12	1:E:264:TYR:HB2	1.63	0.79
1:A:417:GLN:H	1:A:417:GLN:HE21	1.30	0.79
1:B:429:HIS:HD2	1:B:431:GLU:H	1.30	0.79
1:D:448:GLN:HE21	1:D:539:SER:HB3	1.47	0.78
1:B:352:ARG:H	1:B:353:PRO:HD2	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:LYS:HD3	1:B:457:LYS:H	1.48	0.77
1:F:417:GLN:H	1:F:417:GLN:HE21	1.30	0.77
1:C:521:SER:HB3	1:C:525:ARG:NH1	1.99	0.76
1:B:521:SER:HB3	1:B:525:ARG:HH12	1.51	0.76
1:A:444:MET:CE	1:A:486:LEU:HD22	2.15	0.76
1:B:465:ASN:ND2	1:B:467:CYS:H	1.84	0.75
1:A:444:MET:HE1	1:A:486:LEU:HD22	1.67	0.75
1:D:430:HIS:HB2	1:D:523:ASN:HD21	1.51	0.75
1:F:342:LEU:HD22	1:F:366:LEU:HD11	1.69	0.75
1:E:463:ILE:HD12	1:E:504:VAL:HG23	1.68	0.75
1:G:308:LYS:HG3	1:G:309:SER:H	1.51	0.74
1:H:501:GLN:OE1	2:H:903:DTT:S4	2.45	0.74
2:F:903:DTT:H42	2:F:903:DTT:S1	2.27	0.74
1:D:384:LEU:HD21	1:D:496:PHE:HA	1.68	0.74
1:C:465:ASN:HD22	1:C:467:CYS:H	1.34	0.74
1:C:513:LEU:HG	1:C:514:LYS:H	1.52	0.74
1:B:352:ARG:H	1:B:353:PRO:CD	2.00	0.74
1:A:391:PHE:HB3	1:A:407:ALA:HB3	1.68	0.74
1:C:515:ILE:O	1:C:519:ALA:HB3	1.88	0.74
1:F:517:GLU:HG3	1:F:518:GLU:H	1.53	0.74
1:G:465:ASN:O	1:G:509:PRO:HD2	1.86	0.74
1:B:317:ARG:HH21	1:B:317:ARG:HB3	1.53	0.73
1:D:437:LYS:O	1:D:441:GLU:HG3	1.88	0.73
1:A:549:VAL:O	1:A:553:CYS:HB2	1.87	0.73
1:E:396:THR:OG1	1:E:400:ILE:HG12	1.89	0.73
1:E:512:LYS:O	1:E:513:LEU:HB3	1.88	0.73
1:H:465:ASN:HD22	1:H:467:CYS:H	1.36	0.73
1:D:384:LEU:HD22	1:D:494:ARG:NH1	2.04	0.72
1:D:404:VAL:HG21	1:D:416:PRO:HA	1.70	0.72
1:A:395:HIS:HE1	1:A:440:TYR:OH	1.72	0.72
1:F:282:ASP:HB3	1:F:313:VAL:HG22	1.71	0.72
1:H:436:MET:HA	1:H:436:MET:HE2	1.71	0.72
1:A:512:LYS:O	1:A:513:LEU:HB3	1.90	0.72
1:E:272:ARG:HG2	1:E:272:ARG:HH11	1.54	0.72
1:E:507:ALA:O	1:E:509:PRO:HD3	1.89	0.72
1:H:485:LYS:HE2	1:H:537:THR:HB	1.70	0.72
1:E:429:HIS:HD2	1:E:431:GLU:H	1.37	0.72
1:A:555:ALA:HB2	2:A:902:DTT:H2	1.72	0.72
1:H:380:PRO:HD3	2:H:903:DTT:S1	2.30	0.71
1:A:430:HIS:HB2	1:A:523:ASN:HD21	1.54	0.71
1:H:384:LEU:HD12	1:H:496:PHE:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:548:GLU:HA	1:E:551:ARG:HB3	1.72	0.71
1:G:417:GLN:H	1:G:417:GLN:NE2	1.88	0.71
1:H:430:HIS:HB2	1:H:523:ASN:ND2	2.06	0.70
1:F:258:ILE:HD12	1:F:264:TYR:HB2	1.74	0.69
1:A:457:LYS:HD3	1:A:457:LYS:N	2.07	0.69
1:D:417:GLN:H	1:D:417:GLN:HE21	1.40	0.69
1:A:254:THR:HG21	1:A:258:ILE:HG13	1.75	0.69
1:D:501:GLN:HE21	1:D:509:PRO:HB2	1.58	0.68
1:F:476:THR:OG1	1:F:490:VAL:HG13	1.94	0.68
1:G:514:LYS:HD2	1:G:514:LYS:O	1.93	0.68
1:H:533:ARG:HG2	1:H:533:ARG:HH21	1.59	0.68
1:A:465:ASN:O	1:A:509:PRO:HD2	1.93	0.68
1:C:517:GLU:HG3	1:C:518:GLU:H	1.59	0.68
1:E:559:PHE:CE2	1:F:348:PRO:HD3	2.29	0.68
1:A:457:LYS:H	1:A:457:LYS:CD	2.07	0.68
1:C:351:ALA:O	1:C:352:ARG:HB2	1.92	0.67
1:A:510:THR:HG23	1:A:511:CYS:SG	2.34	0.67
1:F:404:VAL:HG11	1:F:419:LEU:HD23	1.76	0.67
1:G:282:ASP:HB3	1:G:313:VAL:HG23	1.77	0.67
1:B:528:GLU:HA	1:B:531:VAL:HG12	1.76	0.67
1:H:429:HIS:HD2	1:H:431:GLU:H	1.42	0.67
1:D:317:ARG:HB3	1:D:317:ARG:HH21	1.60	0.67
1:G:430:HIS:HB2	1:G:523:ASN:HD21	1.59	0.67
1:G:513:LEU:HD12	1:G:514:LYS:N	2.09	0.67
1:C:243:VAL:HG23	1:D:564:MET:SD	2.35	0.66
1:H:352:ARG:H	1:H:353:PRO:CD	2.07	0.66
1:H:476:THR:OG1	1:H:490:VAL:HG13	1.95	0.66
1:A:243:VAL:HG22	1:A:367:VAL:HG22	1.78	0.66
1:B:282:ASP:HB3	1:B:313:VAL:HG22	1.78	0.66
1:D:282:ASP:HB3	1:D:313:VAL:HG22	1.76	0.66
1:E:457:LYS:HD3	1:E:457:LYS:N	2.10	0.66
1:H:317:ARG:HB3	1:H:317:ARG:NH2	2.08	0.66
1:G:549:VAL:O	1:G:553:CYS:HB2	1.95	0.66
1:A:317:ARG:HB3	1:A:317:ARG:NH2	2.11	0.66
1:B:465:ASN:C	1:B:465:ASN:HD22	1.98	0.66
1:E:258:ILE:CD1	1:E:264:TYR:HB2	2.26	0.65
1:A:254:THR:CG2	1:A:258:ILE:HG13	2.26	0.65
1:A:463:ILE:HD12	1:A:504:VAL:HG23	1.77	0.65
1:F:352:ARG:H	1:F:353:PRO:HD2	1.62	0.65
1:G:317:ARG:HH21	1:G:317:ARG:HB3	1.60	0.65
1:C:501:GLN:HE21	1:C:508:ALA:HB1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:TYR:HE1	1:E:266:ARG:HH12	1.43	0.65
1:A:404:VAL:HG21	1:A:416:PRO:HA	1.77	0.65
1:C:465:ASN:HD22	1:C:465:ASN:C	2.00	0.65
1:D:457:LYS:HD3	1:D:457:LYS:N	2.11	0.65
1:C:444:MET:HE1	1:C:486:LEU:HD22	1.79	0.65
1:D:272:ARG:HH11	1:D:272:ARG:HG2	1.61	0.65
1:C:429:HIS:HD2	1:C:431:GLU:H	1.44	0.64
1:A:313:VAL:HG12	1:A:340:LEU:HD11	1.78	0.64
1:C:342:LEU:HD22	1:C:368:ILE:HG12	1.79	0.64
1:C:352:ARG:N	1:C:353:PRO:CD	2.59	0.64
1:E:515:ILE:HG23	1:E:519:ALA:HB2	1.78	0.64
1:F:428:TYR:CD1	1:F:436:MET:HG2	2.33	0.64
1:G:507:ALA:O	1:G:509:PRO:HD3	1.97	0.64
1:A:282:ASP:HB3	1:A:313:VAL:HG23	1.79	0.64
1:C:514:LYS:HG3	1:C:515:ILE:H	1.62	0.64
1:D:348:PRO:HD3	1:D:365:LEU:HD22	1.78	0.64
1:F:501:GLN:HE21	1:F:508:ALA:CB	2.05	0.64
1:A:441:GLU:HG2	1:A:533:ARG:HD2	1.79	0.64
1:G:404:VAL:HG21	1:G:416:PRO:HA	1.80	0.64
1:B:282:ASP:HB3	1:B:313:VAL:CG2	2.28	0.64
1:E:564:MET:HG2	1:F:241:CYS:HB2	1.80	0.63
1:H:517:GLU:O	1:H:521:SER:HB2	1.99	0.63
1:G:457:LYS:H	1:G:457:LYS:CD	2.06	0.63
1:E:457:LYS:H	1:E:457:LYS:CD	2.10	0.63
1:H:457:LYS:H	1:H:457:LYS:CD	2.05	0.63
1:B:521:SER:HB3	1:B:525:ARG:NH1	2.14	0.63
1:C:451:GLY:HA3	1:D:362:THR:HG22	1.80	0.63
1:D:384:LEU:CD2	1:D:496:PHE:HA	2.28	0.63
1:H:351:ALA:O	1:H:352:ARG:HB2	1.97	0.63
1:D:507:ALA:O	1:D:509:PRO:HD3	1.98	0.62
1:E:521:SER:O	1:E:524:THR:HG22	1.99	0.62
1:E:238:ASP:O	1:E:372:PRO:HD2	2.00	0.62
2:F:900:DTT:S4	2:F:900:DTT:O2	2.58	0.62
1:H:238:ASP:O	1:H:372:PRO:HD2	1.98	0.62
1:H:352:ARG:N	1:H:353:PRO:CD	2.62	0.62
1:A:296:ILE:HD11	1:B:478:PHE:HB2	1.81	0.62
1:C:317:ARG:HH21	1:C:317:ARG:HB3	1.65	0.62
1:F:317:ARG:HB3	1:F:317:ARG:NH2	2.14	0.62
1:D:457:LYS:H	1:D:457:LYS:CD	2.11	0.62
1:F:393:ILE:HG12	1:F:404:VAL:HG12	1.81	0.62
1:A:317:ARG:HB3	1:A:317:ARG:HH21	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:ASP:O	1:B:372:PRO:HD2	2.00	0.62
1:C:457:LYS:H	1:C:457:LYS:CD	2.01	0.62
1:G:550:SER:HB2	1:G:556:LEU:HD22	1.81	0.62
1:E:465:ASN:C	1:E:465:ASN:HD22	2.03	0.61
1:F:457:LYS:H	1:F:457:LYS:CD	2.07	0.61
1:G:417:GLN:HE21	1:G:417:GLN:N	1.95	0.61
1:H:257:SER:O	1:H:261:VAL:HG23	2.00	0.61
1:B:272:ARG:HH11	1:B:272:ARG:HG2	1.66	0.61
1:D:510:THR:HG23	1:D:511:CYS:SG	2.40	0.61
1:E:395:HIS:CE1	1:E:424:ILE:HG21	2.35	0.61
1:D:514:LYS:HE2	1:D:519:ALA:HB3	1.82	0.61
1:H:521:SER:HB3	1:H:525:ARG:NH1	2.12	0.61
1:A:479:VAL:HG11	1:A:538:VAL:HG21	1.83	0.61
1:B:546:LYS:O	1:B:549:VAL:HG12	2.00	0.61
1:C:412:LEU:O	1:C:463:ILE:HB	2.00	0.61
1:C:502:CYS:N	2:C:903:DTT:S1	2.71	0.61
1:G:317:ARG:HB3	1:G:317:ARG:NH2	2.14	0.61
1:H:436:MET:HA	1:H:436:MET:CE	2.31	0.61
1:E:430:HIS:HB2	1:E:523:ASN:HD21	1.65	0.61
1:F:316:ARG:HB3	1:F:335:TYR:CE1	2.35	0.61
1:G:559:PHE:CE2	1:H:348:PRO:HD3	2.36	0.61
1:E:509:PRO:O	1:E:510:THR:HG22	2.02	0.60
1:E:485:LYS:HE2	1:E:537:THR:HB	1.83	0.60
2:H:903:DTT:S1	2:H:903:DTT:C4	2.81	0.60
1:E:308:LYS:HG3	1:E:309:SER:H	1.66	0.60
1:F:347:ALA:HB2	1:F:365:LEU:HD13	1.83	0.60
1:F:546:LYS:O	1:F:549:VAL:HG12	2.01	0.60
1:E:465:ASN:O	1:E:509:PRO:HD2	2.00	0.60
1:E:417:GLN:H	1:E:417:GLN:HE21	1.50	0.60
1:H:248:ASP:OD1	1:H:250:ILE:HG12	2.02	0.60
1:B:287:ALA:O	1:B:290:ILE:HD13	2.02	0.60
1:D:465:ASN:ND2	1:D:467:CYS:H	1.99	0.60
1:G:262:LEU:HD22	1:G:317:ARG:HA	1.82	0.60
1:H:417:GLN:H	1:H:417:GLN:NE2	1.96	0.60
1:A:548:GLU:HA	1:A:551:ARG:CB	2.32	0.60
1:G:378:LYS:HD2	1:G:378:LYS:N	2.17	0.60
1:C:282:ASP:HB3	1:C:313:VAL:CG2	2.32	0.60
1:G:484:ARG:HG2	1:G:484:ARG:HH11	1.67	0.60
1:D:316:ARG:HB3	1:D:335:TYR:CE1	2.37	0.59
2:F:903:DTT:S1	2:F:903:DTT:C4	2.89	0.59
1:G:444:MET:CE	1:G:486:LEU:HD22	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:395:HIS:HE1	1:G:440:TYR:OH	1.85	0.59
1:B:312:CYS:SG	1:B:373:ILE:HD11	2.42	0.59
1:F:287:ALA:O	1:F:290:ILE:HD13	2.02	0.59
1:E:437:LYS:O	1:E:441:GLU:HG3	2.03	0.59
1:G:457:LYS:HD3	1:G:457:LYS:N	2.07	0.59
1:B:352:ARG:N	1:B:353:PRO:CD	2.64	0.59
1:F:342:LEU:CD2	1:F:368:ILE:HG12	2.32	0.59
1:B:248:ASP:OD1	1:B:250:ILE:HG12	2.03	0.59
1:F:444:MET:HE1	1:F:486:LEU:HB2	1.84	0.59
1:B:317:ARG:HB3	1:B:317:ARG:NH2	2.17	0.59
1:B:391:PHE:HB3	1:B:407:ALA:HB3	1.85	0.59
1:C:469:VAL:HG23	1:C:471:LEU:HD13	1.85	0.59
1:H:444:MET:HE1	1:H:486:LEU:HD22	1.84	0.59
1:H:465:ASN:HD22	1:H:465:ASN:C	2.06	0.59
1:A:272:ARG:HH11	1:A:272:ARG:CG	2.13	0.58
1:F:463:ILE:HD12	1:F:504:VAL:HG12	1.85	0.58
1:F:384:LEU:HD23	1:F:385:SER:N	2.18	0.58
1:D:395:HIS:HD2	1:D:396:THR:O	1.85	0.58
1:A:429:HIS:HD2	1:A:431:GLU:H	1.50	0.58
1:A:551:ARG:HH21	1:A:552:ARG:HB3	1.68	0.58
1:C:465:ASN:ND2	1:C:467:CYS:HB2	2.11	0.58
1:E:503:ASN:HD22	1:E:506:GLU:HB3	1.69	0.58
1:A:453:SER:O	1:A:454:PHE:HB3	2.02	0.58
1:C:513:LEU:HG	1:C:514:LYS:N	2.17	0.58
1:E:515:ILE:O	1:E:519:ALA:HB3	2.03	0.58
1:F:521:SER:HB3	1:F:525:ARG:NH1	2.09	0.58
1:A:441:GLU:HG2	1:A:533:ARG:CD	2.34	0.58
1:B:480:ASN:HB2	1:B:487:GLU:OE2	2.03	0.58
1:G:465:ASN:C	1:G:465:ASN:HD22	2.07	0.58
1:D:503:ASN:HD22	1:D:506:GLU:HB3	1.69	0.58
1:C:241:CYS:HG	1:C:369:CYS:HG	1.43	0.58
1:F:314:MET:HG2	1:F:415:LEU:HD11	1.84	0.58
1:A:479:VAL:HG11	1:A:538:VAL:CG2	2.34	0.57
1:C:533:ARG:HG2	1:C:533:ARG:HH21	1.68	0.57
1:E:461:PHE:HB2	1:E:471:LEU:HD22	1.85	0.57
1:F:481:PRO:O	1:F:484:ARG:NH1	2.37	0.57
1:C:348:PRO:HD3	1:D:559:PHE:CE2	2.40	0.57
1:D:236:LYS:HD2	1:D:237:GLU:N	2.20	0.57
1:C:287:ALA:O	1:C:290:ILE:HD13	2.04	0.57
1:E:479:VAL:HG11	1:E:538:VAL:CG2	2.34	0.57
1:F:396:THR:OG1	1:F:400:ILE:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:ILE:HG22	1:F:342:LEU:HD11	1.87	0.57
1:H:545:VAL:HG12	1:H:546:LYS:H	1.69	0.57
1:C:241:CYS:HB2	1:D:564:MET:HG3	1.85	0.57
1:C:513:LEU:CG	1:C:514:LYS:H	2.17	0.57
1:D:517:GLU:HG3	1:D:518:GLU:H	1.70	0.57
1:D:258:ILE:HD13	1:D:258:ILE:O	2.05	0.56
1:E:296:ILE:HD11	1:F:478:PHE:HB2	1.86	0.56
1:A:509:PRO:O	1:A:510:THR:HG22	2.06	0.56
1:C:282:ASP:HB3	1:C:313:VAL:HG22	1.87	0.56
1:D:253:TYR:HE1	1:D:266:ARG:HH12	1.54	0.56
1:D:384:LEU:HB3	1:D:494:ARG:NH2	2.20	0.56
1:F:317:ARG:HB3	1:F:317:ARG:HH21	1.70	0.56
1:G:441:GLU:HG2	1:G:533:ARG:HD2	1.86	0.56
1:H:316:ARG:HB3	1:H:335:TYR:CE1	2.40	0.56
1:H:395:HIS:HD2	1:H:396:THR:O	1.87	0.56
1:H:465:ASN:HD22	1:H:466:GLY:N	2.04	0.56
1:A:559:PHE:CE2	1:B:348:PRO:HD3	2.39	0.56
1:D:465:ASN:O	1:D:508:ALA:HA	2.06	0.56
1:E:444:MET:HE1	1:E:486:LEU:HD22	1.88	0.56
1:A:246:MET:HB2	1:A:364:MET:HB3	1.88	0.56
1:A:460:ARG:HA	1:A:469:VAL:O	2.06	0.56
1:D:378:LYS:O	1:D:502:CYS:SG	2.64	0.56
1:D:518:GLU:O	1:D:522:ARG:HB3	2.05	0.56
1:F:465:ASN:HD22	1:F:465:ASN:C	2.09	0.56
1:D:501:GLN:HG3	1:D:509:PRO:HG2	1.86	0.56
1:E:253:TYR:CG	1:E:254:THR:N	2.74	0.56
1:G:463:ILE:HD12	1:G:504:VAL:HG23	1.86	0.56
1:H:379:VAL:O	1:H:382:GLU:HB2	2.06	0.56
1:C:272:ARG:HH11	1:C:272:ARG:CG	2.14	0.56
2:C:901:DTT:S4	2:C:901:DTT:H12	2.45	0.56
1:B:351:ALA:O	1:B:352:ARG:HB2	2.06	0.56
1:G:308:LYS:HG3	1:G:309:SER:N	2.21	0.56
1:D:254:THR:HG21	1:D:258:ILE:HG13	1.87	0.55
1:H:240:PHE:CD1	1:H:258:ILE:HG12	2.40	0.55
1:A:507:ALA:O	1:A:509:PRO:HD3	2.06	0.55
1:B:465:ASN:HD22	1:B:467:CYS:H	1.51	0.55
1:F:378:LYS:N	1:F:378:LYS:HD2	2.21	0.55
1:H:532:LYS:O	1:H:532:LYS:HD3	2.06	0.55
1:A:294:ILE:HG13	1:A:295:PRO:HD2	1.88	0.55
2:B:901:DTT:S1	2:B:901:DTT:S4	3.00	0.55
1:F:384:LEU:HD12	1:F:496:PHE:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:HG22	1:A:334:SER:N	2.22	0.55
1:G:555:ALA:HB2	2:G:902:DTT:H2	1.89	0.55
1:C:444:MET:CE	1:C:486:LEU:HD22	2.36	0.55
1:A:417:GLN:H	1:A:417:GLN:NE2	2.02	0.55
1:G:548:GLU:HA	1:G:551:ARG:CB	2.36	0.55
1:H:465:ASN:HA	1:H:507:ALA:HA	1.89	0.55
1:E:348:PRO:HD3	1:E:365:LEU:HD22	1.88	0.55
1:A:550:SER:HB2	1:A:556:LEU:HD22	1.89	0.54
1:C:517:GLU:CG	1:C:518:GLU:H	2.18	0.54
1:E:550:SER:HB2	1:E:556:LEU:CD2	2.37	0.54
1:B:532:LYS:HD3	1:B:532:LYS:O	2.07	0.54
1:E:342:LEU:HD22	1:E:366:LEU:HD11	1.88	0.54
1:F:430:HIS:HB2	1:F:523:ASN:ND2	2.23	0.54
1:G:465:ASN:ND2	1:G:467:CYS:H	2.05	0.54
1:H:401:ILE:HD13	1:H:419:LEU:HG	1.89	0.54
1:H:513:LEU:HG	1:H:514:LYS:N	2.22	0.54
1:B:378:LYS:N	1:B:378:LYS:HD2	2.21	0.54
1:B:384:LEU:HD23	1:B:385:SER:N	2.22	0.54
1:B:430:HIS:HB2	1:B:523:ASN:ND2	2.22	0.54
1:D:509:PRO:O	1:D:510:THR:HG22	2.07	0.54
1:B:412:LEU:O	1:B:463:ILE:HB	2.08	0.54
1:C:517:GLU:O	1:C:521:SER:HB2	2.08	0.54
1:D:439:THR:O	1:D:443:VAL:HG23	2.08	0.54
1:G:522:ARG:HE	1:G:522:ARG:HA	1.73	0.54
1:A:503:ASN:ND2	1:A:506:GLU:HB3	2.22	0.54
1:F:517:GLU:O	1:F:521:SER:HB2	2.08	0.54
1:D:515:ILE:HG22	1:D:519:ALA:HB2	1.90	0.54
1:F:463:ILE:HG12	1:F:467:CYS:O	2.07	0.54
1:A:430:HIS:CE1	1:A:431:GLU:HG3	2.42	0.54
1:C:546:LYS:O	1:C:549:VAL:HG12	2.07	0.54
1:G:272:ARG:HH11	1:G:272:ARG:HG2	1.72	0.54
1:C:241:CYS:HB2	1:D:564:MET:CG	2.38	0.53
1:G:444:MET:HE1	1:G:486:LEU:HD22	1.90	0.53
1:B:254:THR:HG22	1:B:255:THR:O	2.08	0.53
1:F:513:LEU:HG	1:F:514:LYS:N	2.24	0.53
1:A:272:ARG:HG2	1:A:272:ARG:NH1	2.19	0.53
1:E:384:LEU:N	1:E:384:LEU:HD12	2.23	0.53
1:B:258:ILE:HD12	1:B:264:TYR:HB2	1.91	0.53
1:B:347:ALA:HB2	1:B:365:LEU:HD13	1.89	0.53
1:E:548:GLU:HA	1:E:551:ARG:CB	2.39	0.53
1:B:241:CYS:HG	1:B:369:CYS:CB	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:LEU:HD22	1:E:317:ARG:HA	1.91	0.53
1:E:404:VAL:CG2	1:E:416:PRO:HA	2.37	0.53
1:F:528:GLU:O	1:F:532:LYS:HB2	2.08	0.53
1:G:465:ASN:HD22	1:G:467:CYS:H	1.56	0.53
1:H:258:ILE:HD12	1:H:264:TYR:HB2	1.91	0.53
1:H:376:SER:OG	1:H:410:SER:HB3	2.09	0.53
1:B:412:LEU:HD13	1:B:461:PHE:CE1	2.44	0.53
1:D:526:ILE:O	1:D:530:ILE:HG13	2.09	0.53
1:D:281:LYS:HE2	1:D:418:ASP:OD1	2.10	0.52
1:F:429:HIS:HD2	1:F:431:GLU:H	1.54	0.52
1:H:397:ALA:HB2	1:H:486:LEU:O	2.09	0.52
1:H:548:GLU:HG3	1:H:551:ARG:NH2	2.23	0.52
1:A:236:LYS:HD2	1:A:237:GLU:N	2.24	0.52
1:B:282:ASP:CB	1:B:313:VAL:HG22	2.38	0.52
1:C:395:HIS:HD2	1:C:396:THR:O	1.93	0.52
1:F:352:ARG:H	1:F:353:PRO:HD3	1.73	0.52
1:A:444:MET:HE3	1:A:486:LEU:HD22	1.89	0.52
1:D:378:LYS:N	1:D:378:LYS:HD2	2.24	0.52
1:A:437:LYS:O	1:A:441:GLU:HG3	2.10	0.52
1:B:432:ASP:O	1:B:435:VAL:HG12	2.09	0.52
1:B:473:THR:OG1	1:B:493:HIS:HD2	1.93	0.52
1:C:251:VAL:HG13	1:C:269:TRP:O	2.09	0.52
1:C:433:LEU:HD12	1:C:523:ASN:ND2	2.25	0.52
1:B:469:VAL:HG23	1:B:471:LEU:HD13	1.92	0.52
1:B:501:GLN:NE2	1:B:508:ALA:HB1	2.19	0.52
1:D:258:ILE:CD1	1:D:264:TYR:HB2	2.36	0.52
1:H:378:LYS:HD2	1:H:378:LYS:N	2.25	0.52
1:B:517:GLU:HG3	1:B:518:GLU:H	1.75	0.52
1:A:484:ARG:HE	1:A:540:ARG:HB2	1.73	0.52
1:D:308:LYS:HG3	1:D:309:SER:H	1.75	0.52
1:E:549:VAL:O	1:E:553:CYS:HB2	2.10	0.52
1:G:445:LYS:O	1:G:448:GLN:HB2	2.10	0.52
1:D:503:ASN:ND2	1:D:506:GLU:HB3	2.25	0.52
1:E:253:TYR:HE1	1:E:266:ARG:NH1	2.08	0.52
1:G:441:GLU:HG2	1:G:533:ARG:CD	2.40	0.52
1:G:544:THR:HA	1:G:547:GLN:HG2	1.91	0.52
1:H:352:ARG:N	1:H:353:PRO:HD2	2.15	0.52
1:B:457:LYS:H	1:B:457:LYS:CD	2.20	0.52
1:C:417:GLN:H	1:C:417:GLN:NE2	2.02	0.52
1:H:460:ARG:HA	1:H:469:VAL:O	2.10	0.52
1:E:239:SER:HB2	1:E:371:THR:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:513:LEU:HG	1:F:514:LYS:H	1.74	0.51
1:A:511:CYS:O	1:A:512:LYS:HG2	2.11	0.51
1:G:503:ASN:HD22	1:G:506:GLU:HB3	1.75	0.51
1:E:391:PHE:HB3	1:E:407:ALA:HB3	1.90	0.51
1:B:465:ASN:HD22	1:B:466:GLY:N	2.08	0.51
1:D:433:LEU:HD12	1:D:523:ASN:CG	2.30	0.51
2:D:900:DTT:S4	2:D:900:DTT:H12	2.50	0.51
1:E:236:LYS:HD2	1:E:237:GLU:N	2.25	0.51
1:E:248:ASP:OD1	1:E:250:ILE:HG12	2.11	0.51
1:E:398:THR:HA	1:E:531:VAL:HG23	1.92	0.51
1:E:481:PRO:HG2	1:E:482:TRP:CE3	2.45	0.51
1:D:384:LEU:HD22	1:D:494:ARG:CZ	2.39	0.51
1:G:485:LYS:HE3	1:G:537:THR:HB	1.92	0.51
1:C:473:THR:OG1	1:C:493:HIS:HD2	1.93	0.51
1:D:444:MET:HE2	1:D:444:MET:HA	1.93	0.51
1:F:339:ARG:HH21	2:F:900:DTT:H11	1.76	0.51
1:D:463:ILE:HG12	1:D:467:CYS:O	2.10	0.51
1:D:259:THR:O	1:D:263:GLY:HA2	2.11	0.51
1:F:272:ARG:HH11	1:F:272:ARG:CG	2.19	0.51
1:G:547:GLN:C	1:G:549:VAL:H	2.13	0.51
1:D:238:ASP:O	1:D:372:PRO:HD2	2.10	0.51
1:D:548:GLU:HA	1:D:551:ARG:HB3	1.92	0.51
1:E:378:LYS:HD2	1:E:378:LYS:N	2.26	0.51
1:F:238:ASP:O	1:F:372:PRO:HD2	2.11	0.50
1:F:517:GLU:HG3	1:F:518:GLU:N	2.22	0.50
1:H:240:PHE:CE2	1:H:370:ALA:HB3	2.46	0.50
1:C:246:MET:HB2	1:C:364:MET:HB3	1.92	0.50
1:H:470:LEU:HB2	1:H:497:GLN:HB3	1.93	0.50
1:B:412:LEU:HD13	1:B:461:PHE:HE1	1.75	0.50
1:B:513:LEU:HG	1:B:514:LYS:N	2.26	0.50
1:A:362:THR:HG22	1:B:451:GLY:HA3	1.94	0.50
1:A:522:ARG:HH21	1:A:525:ARG:HD2	1.77	0.50
1:C:290:ILE:HG22	1:C:342:LEU:HD11	1.93	0.50
1:E:473:THR:HG22	1:E:474:GLU:N	2.26	0.50
1:B:515:ILE:O	1:B:519:ALA:HB3	2.12	0.50
1:B:517:GLU:O	1:B:521:SER:HB2	2.11	0.50
1:E:486:LEU:HD21	1:E:489:VAL:HG23	1.94	0.50
1:F:352:ARG:N	1:F:353:PRO:CD	2.64	0.50
1:B:465:ASN:HD21	1:B:467:CYS:HB2	1.76	0.50
1:C:379:VAL:HB	1:C:380:PRO:HD2	1.92	0.50
1:D:430:HIS:CB	1:D:523:ASN:HD21	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:518:GLU:O	1:F:522:ARG:HB3	2.12	0.50
1:C:476:THR:OG1	1:C:490:VAL:HG13	2.12	0.50
1:G:509:PRO:O	1:G:510:THR:HG22	2.12	0.50
1:E:447:GLY:O	1:E:540:ARG:NH2	2.44	0.50
1:E:479:VAL:HG11	1:E:538:VAL:HG21	1.94	0.50
1:H:308:LYS:HG3	1:H:309:SER:N	2.27	0.50
1:C:342:LEU:CD2	1:C:368:ILE:HG12	2.42	0.50
1:C:482:TRP:HB3	1:D:275:ILE:HD13	1.93	0.50
1:H:546:LYS:O	1:H:549:VAL:HG12	2.12	0.50
1:A:564:MET:CG	1:B:241:CYS:HB2	2.42	0.49
1:D:501:GLN:HG3	1:D:509:PRO:CG	2.42	0.49
1:F:517:GLU:CG	1:F:518:GLU:H	2.18	0.49
1:A:313:VAL:HG12	1:A:340:LEU:CD1	2.42	0.49
1:A:378:LYS:HD2	1:A:378:LYS:N	2.26	0.49
1:A:380:PRO:HD3	2:A:903:DTT:S1	2.52	0.49
1:A:482:TRP:CD1	1:B:275:ILE:HG12	2.47	0.49
1:A:485:LYS:HE2	1:A:537:THR:HB	1.94	0.49
1:E:272:ARG:HG2	1:E:272:ARG:NH1	2.27	0.49
1:C:339:ARG:HH21	2:C:900:DTT:H11	1.77	0.49
1:A:499:PRO:HG2	1:A:501:GLN:O	2.12	0.49
1:F:473:THR:OG1	1:F:493:HIS:HD2	1.95	0.49
1:G:533:ARG:O	1:G:536:GLU:HB2	2.12	0.49
1:D:383:ILE:CG2	1:D:384:LEU:N	2.75	0.49
1:D:465:ASN:HD22	1:D:466:GLY:N	2.10	0.49
1:D:469:VAL:HG23	1:D:471:LEU:HD13	1.94	0.49
1:D:484:ARG:HE	1:D:540:ARG:HB2	1.78	0.49
1:D:384:LEU:HD13	1:D:494:ARG:HH22	1.77	0.49
1:E:550:SER:HB2	1:E:556:LEU:HD22	1.95	0.49
1:G:267:ASP:HB2	1:G:270:LEU:HG	1.93	0.49
1:H:517:GLU:HG3	1:H:518:GLU:H	1.77	0.49
1:C:347:ALA:HB2	1:C:365:LEU:HD13	1.95	0.49
1:E:290:ILE:HG22	1:E:342:LEU:HD11	1.95	0.49
1:E:511:CYS:O	1:E:512:LYS:HG2	2.13	0.49
1:C:258:ILE:O	1:C:258:ILE:HD13	2.12	0.49
1:D:513:LEU:HD12	1:D:514:LYS:N	2.28	0.49
1:H:430:HIS:HB2	1:H:523:ASN:HD21	1.78	0.49
1:C:430:HIS:HB2	1:C:523:ASN:ND2	2.28	0.48
1:D:447:GLY:O	1:D:540:ARG:NH2	2.44	0.48
1:F:417:GLN:H	1:F:417:GLN:NE2	2.04	0.48
1:G:267:ASP:HB2	1:G:270:LEU:CD1	2.43	0.48
1:E:367:VAL:HG21	1:F:563:LEU:CD2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:528:GLU:O	1:E:532:LYS:HB2	2.13	0.48
1:H:469:VAL:HG23	1:H:471:LEU:HD13	1.95	0.48
1:A:287:ALA:O	1:A:290:ILE:HD13	2.14	0.48
1:C:242:CYS:SG	1:C:244:ILE:HD11	2.53	0.48
1:E:342:LEU:CD2	1:E:368:ILE:HG12	2.43	0.48
1:C:282:ASP:CB	1:C:313:VAL:HG22	2.43	0.48
1:E:473:THR:OG1	1:E:493:HIS:CD2	2.67	0.48
1:F:272:ARG:HG2	1:F:272:ARG:NH1	2.19	0.48
1:D:465:ASN:HB2	1:D:509:PRO:HD2	1.94	0.48
1:E:392:ALA:H	1:E:405:ASP:HB2	1.79	0.48
1:G:444:MET:HE2	1:G:444:MET:HA	1.95	0.48
1:C:378:LYS:HD3	1:C:387:LYS:HZ1	1.79	0.48
1:C:417:GLN:HE21	1:C:417:GLN:N	2.02	0.48
1:D:311:PHE:HE2	1:D:342:LEU:HG	1.78	0.48
1:E:510:THR:HG23	1:E:511:CYS:N	2.28	0.48
1:F:458:PRO:HG3	1:F:472:GLU:HB3	1.94	0.48
1:H:342:LEU:HD22	1:H:366:LEU:HD11	1.94	0.48
1:H:465:ASN:HD21	1:H:467:CYS:H	1.59	0.48
1:C:307:ALA:HB1	1:D:571:ASP:OD1	2.14	0.48
1:E:473:THR:OG1	1:E:493:HIS:HD2	1.96	0.48
1:G:316:ARG:HB3	1:G:335:TYR:CE1	2.49	0.48
1:A:344:PHE:HB3	1:A:364:MET:HE1	1.94	0.48
1:B:444:MET:HE3	1:B:486:LEU:HB2	1.95	0.48
1:F:417:GLN:HE21	1:F:417:GLN:N	2.05	0.48
1:G:447:GLY:O	1:G:540:ARG:NH2	2.46	0.48
1:H:518:GLU:O	1:H:522:ARG:HB3	2.14	0.48
1:A:484:ARG:HG2	1:A:484:ARG:HH11	1.79	0.48
1:D:344:PHE:HB3	1:D:364:MET:HE2	1.96	0.48
1:E:461:PHE:CB	1:E:471:LEU:HD22	2.43	0.48
1:F:521:SER:O	1:F:524:THR:HG22	2.14	0.48
1:A:333:VAL:HG22	1:A:334:SER:H	1.77	0.47
1:B:513:LEU:HG	1:B:514:LYS:H	1.79	0.47
1:C:384:LEU:HD23	1:C:385:SER:N	2.29	0.47
1:C:522:ARG:HA	1:C:522:ARG:HE	1.79	0.47
1:D:550:SER:HA	1:D:553:CYS:HB2	1.96	0.47
1:F:522:ARG:HE	1:F:522:ARG:HA	1.79	0.47
1:A:436:MET:CE	1:A:436:MET:HA	2.42	0.47
1:C:380:PRO:HB3	2:C:903:DTT:O2	2.14	0.47
1:E:281:LYS:HE2	1:E:418:ASP:OD1	2.13	0.47
1:G:481:PRO:HG2	1:G:482:TRP:CE3	2.50	0.47
1:E:444:MET:CE	1:E:486:LEU:HD22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:501:GLN:HE21	1:E:509:PRO:HB2	1.79	0.47
1:F:279:HIS:ND1	1:F:280:LEU:N	2.61	0.47
1:B:433:LEU:HD12	1:B:523:ASN:ND2	2.30	0.47
1:D:546:LYS:C	1:D:548:GLU:H	2.18	0.47
1:F:342:LEU:HD22	1:F:368:ILE:HG12	1.96	0.47
1:B:244:ILE:HB	1:B:366:LEU:HB3	1.97	0.47
1:C:380:PRO:HB3	2:C:903:DTT:HO2	1.78	0.47
1:H:384:LEU:HD21	1:H:494:ARG:NH1	2.29	0.47
1:B:436:MET:HA	1:B:436:MET:CE	2.44	0.47
1:E:481:PRO:HG2	1:E:482:TRP:CD2	2.50	0.47
1:G:444:MET:HE3	1:G:486:LEU:HD22	1.96	0.47
1:G:511:CYS:O	1:G:512:LYS:HG2	2.14	0.47
1:D:378:LYS:C	1:D:502:CYS:SG	2.93	0.47
1:D:444:MET:HE1	1:D:486:LEU:HD22	1.95	0.47
1:E:253:TYR:HB2	1:F:556:LEU:HD13	1.96	0.47
1:E:379:VAL:HB	1:E:380:PRO:HD2	1.96	0.47
1:F:402:SER:OG	1:F:403:HIS:CD2	2.68	0.47
1:H:501:GLN:NE2	1:H:510:THR:HG21	2.29	0.47
1:C:342:LEU:HD13	1:C:366:LEU:HD11	1.96	0.47
1:C:238:ASP:O	1:C:372:PRO:HD2	2.15	0.47
1:D:463:ILE:HD12	1:D:504:VAL:CG2	2.35	0.47
1:F:419:LEU:O	1:F:422:ARG:HB2	2.14	0.47
2:H:901:DTT:H12	2:H:901:DTT:H42	1.55	0.47
1:C:315:LEU:HD12	1:C:338:PHE:CD2	2.50	0.47
1:E:441:GLU:HG2	1:E:533:ARG:CD	2.45	0.47
1:G:443:VAL:HG22	1:G:454:PHE:HE1	1.80	0.47
1:G:453:SER:O	1:G:454:PHE:HB3	2.14	0.47
1:E:258:ILE:HD13	1:E:258:ILE:O	2.14	0.46
1:E:294:ILE:HG23	1:E:294:ILE:O	2.15	0.46
1:E:547:GLN:OE1	1:E:547:GLN:HA	2.15	0.46
1:F:395:HIS:HD2	1:F:396:THR:O	1.98	0.46
1:G:252:LEU:HB3	1:H:556:LEU:HD13	1.98	0.46
1:A:417:GLN:HE21	1:A:417:GLN:N	2.05	0.46
1:G:333:VAL:HG22	1:G:334:SER:N	2.30	0.46
1:H:463:ILE:HD12	1:H:504:VAL:HG12	1.97	0.46
1:A:522:ARG:HE	1:A:522:ARG:HA	1.81	0.46
1:B:480:ASN:HB3	1:B:483:SER:OG	2.15	0.46
1:C:542:SER:C	1:C:544:THR:H	2.18	0.46
1:G:395:HIS:CE1	1:G:424:ILE:HG21	2.51	0.46
1:H:424:ILE:HD11	3:H:142:HOH:O	2.15	0.46
1:B:528:GLU:O	1:B:532:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ILE:HG22	1:D:384:LEU:N	2.29	0.46
1:D:465:ASN:HB2	1:D:509:PRO:CD	2.45	0.46
1:E:343:THR:HB	1:E:367:VAL:HB	1.97	0.46
1:F:244:ILE:HD12	1:F:274:PHE:HB2	1.98	0.46
2:A:900:DTT:S4	2:A:900:DTT:H12	2.55	0.46
1:B:525:ARG:HH11	1:B:525:ARG:HG3	1.80	0.46
1:E:435:VAL:O	1:E:438:GLU:HG2	2.16	0.46
1:F:253:TYR:HD2	1:F:254:THR:N	2.13	0.46
1:F:258:ILE:HD13	1:F:258:ILE:O	2.16	0.46
1:F:351:ALA:O	1:F:352:ARG:HB2	2.13	0.46
1:F:457:LYS:HD3	1:F:457:LYS:N	2.11	0.46
1:A:402:SER:OG	1:A:403:HIS:HD2	1.99	0.46
1:G:450:ALA:HB2	1:G:540:ARG:NH1	2.31	0.46
1:H:272:ARG:HG2	1:H:272:ARG:HH11	1.81	0.46
1:H:417:GLN:HE21	1:H:417:GLN:N	2.02	0.46
1:B:476:THR:OG1	1:B:490:VAL:HG13	2.16	0.46
1:B:520:GLN:O	1:B:524:THR:HB	2.16	0.46
2:B:900:DTT:S4	2:B:900:DTT:O2	2.68	0.46
1:E:559:PHE:HE2	1:F:348:PRO:HD3	1.78	0.46
1:G:252:LEU:HB3	1:H:556:LEU:CD1	2.46	0.46
1:A:497:GLN:NE2	1:F:386:GLN:HB2	2.31	0.46
1:C:517:GLU:HG3	1:C:518:GLU:N	2.27	0.46
1:D:547:GLN:C	1:D:549:VAL:H	2.19	0.46
1:H:465:ASN:HD21	1:H:467:CYS:HB2	1.80	0.46
1:A:560:MET:SD	1:B:243:VAL:HG11	2.56	0.46
1:B:533:ARG:HH21	1:B:533:ARG:HG2	1.80	0.46
1:F:352:ARG:HD2	1:F:352:ARG:HA	1.75	0.46
1:B:518:GLU:O	1:B:522:ARG:HB3	2.16	0.46
1:F:515:ILE:O	1:F:519:ALA:HB3	2.16	0.46
1:C:279:HIS:ND1	1:C:280:LEU:N	2.64	0.45
1:G:550:SER:HB2	1:G:556:LEU:CD2	2.46	0.45
1:C:241:CYS:SG	1:C:369:CYS:SG	3.01	0.45
1:D:473:THR:HB	1:D:475:TRP:NE1	2.31	0.45
1:D:521:SER:O	1:D:524:THR:HG22	2.17	0.45
1:H:429:HIS:CD2	1:H:431:GLU:H	2.27	0.45
1:H:513:LEU:HG	1:H:514:LYS:H	1.81	0.45
1:D:555:ALA:HB2	2:D:902:DTT:H2	1.99	0.45
1:E:237:GLU:O	1:E:238:ASP:C	2.55	0.45
1:H:522:ARG:HE	1:H:522:ARG:HA	1.82	0.45
1:A:395:HIS:CD2	1:A:489:VAL:HB	2.52	0.45
1:D:522:ARG:O	1:D:526:ILE:HG12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:ARG:HE	1:B:522:ARG:HA	1.81	0.45
1:C:463:ILE:HD12	1:C:504:VAL:HG12	1.97	0.45
1:F:458:PRO:HA	1:F:471:LEU:O	2.16	0.45
1:G:242:CYS:SG	1:G:244:ILE:HD11	2.57	0.45
1:G:433:LEU:HD23	1:G:433:LEU:HA	1.86	0.45
1:A:244:ILE:HD12	1:A:274:PHE:HB2	1.99	0.45
1:F:409:VAL:HG21	2:F:900:DTT:S1	2.57	0.45
1:G:391:PHE:HB3	1:G:407:ALA:HB3	1.98	0.45
1:G:512:LYS:O	1:G:513:LEU:HB3	2.15	0.45
1:A:279:HIS:HD2	1:A:335:TYR:CD2	2.35	0.45
1:A:513:LEU:HD12	1:A:514:LYS:N	2.32	0.45
1:C:444:MET:HE2	1:C:444:MET:HA	1.98	0.45
1:D:515:ILE:CG2	1:D:519:ALA:HB2	2.47	0.45
1:G:429:HIS:HD2	1:G:431:GLU:H	1.64	0.45
1:H:533:ARG:HH21	1:H:533:ARG:CG	2.29	0.45
1:B:308:LYS:HG3	1:B:309:SER:H	1.82	0.45
1:D:272:ARG:HG2	1:D:272:ARG:NH1	2.30	0.45
1:D:429:HIS:HD2	1:D:431:GLU:H	1.64	0.45
1:A:395:HIS:CE1	1:A:440:TYR:OH	2.61	0.45
1:A:503:ASN:HD22	1:A:506:GLU:HB3	1.82	0.45
1:C:277:PHE:O	1:C:315:LEU:HA	2.17	0.45
1:E:465:ASN:ND2	1:E:467:CYS:H	2.15	0.45
1:F:236:LYS:HD2	1:F:237:GLU:N	2.31	0.45
1:F:281:LYS:NZ	1:F:415:LEU:HD12	2.32	0.45
1:G:544:THR:HA	1:G:547:GLN:CG	2.47	0.45
1:H:282:ASP:HB3	1:H:313:VAL:HG22	2.00	0.45
1:H:512:LYS:HB3	1:H:513:LEU:H	1.41	0.44
1:A:515:ILE:O	1:A:519:ALA:HB3	2.17	0.44
1:B:445:LYS:O	1:B:448:GLN:HB2	2.17	0.44
1:B:465:ASN:ND2	1:B:465:ASN:C	2.66	0.44
1:E:395:HIS:ND1	1:E:424:ILE:HG21	2.31	0.44
1:F:248:ASP:OD1	1:F:250:ILE:HG12	2.18	0.44
1:B:519:ALA:O	1:B:523:ASN:HB2	2.16	0.44
1:D:460:ARG:HG3	1:D:470:LEU:CD2	2.47	0.44
1:E:412:LEU:O	1:E:463:ILE:HB	2.17	0.44
1:F:390:LYS:HA	1:F:493:HIS:O	2.18	0.44
1:G:471:LEU:HD23	1:G:493:HIS:CD2	2.53	0.44
1:G:527:LYS:O	1:G:531:VAL:HG12	2.17	0.44
1:D:481:PRO:HG2	1:D:482:TRP:CE3	2.52	0.44
1:E:394:ARG:HB3	1:E:403:HIS:HB2	1.99	0.44
1:H:308:LYS:HG3	1:H:309:SER:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:485:LYS:HE2	1:H:537:THR:CB	2.44	0.44
1:A:290:ILE:HG13	1:B:482:TRP:HZ3	1.83	0.44
1:A:393:ILE:HG12	1:A:404:VAL:HG12	1.98	0.44
1:D:548:GLU:HA	1:D:551:ARG:CB	2.48	0.44
1:E:344:PHE:CE1	1:E:366:LEU:HD13	2.52	0.44
1:A:564:MET:HG2	1:B:255:THR:CG2	2.47	0.44
1:G:253:TYR:HE1	1:G:266:ARG:HH12	1.65	0.44
1:G:384:LEU:HD12	1:G:384:LEU:N	2.32	0.44
1:B:289:GLN:HG3	1:B:311:PHE:CD2	2.52	0.44
1:B:542:SER:C	1:B:544:THR:H	2.20	0.44
1:B:544:THR:HG23	1:B:548:GLU:CD	2.37	0.44
1:G:513:LEU:HD12	1:G:513:LEU:C	2.38	0.44
1:A:482:TRP:HB3	1:B:275:ILE:CD1	2.48	0.44
1:A:433:LEU:HA	1:A:433:LEU:HD23	1.77	0.44
1:C:367:VAL:HG21	1:D:563:LEU:HG	2.00	0.44
1:C:545:VAL:HG12	1:C:546:LYS:H	1.82	0.44
1:D:404:VAL:HG23	1:D:416:PRO:HG3	2.00	0.44
1:E:395:HIS:C	1:E:395:HIS:CD2	2.91	0.44
1:A:527:LYS:O	1:A:531:VAL:HG12	2.18	0.43
1:A:564:MET:HG3	1:B:241:CYS:HB2	1.99	0.43
1:B:394:ARG:HG3	1:B:490:VAL:HB	1.99	0.43
1:B:525:ARG:NH1	1:B:525:ARG:HG3	2.32	0.43
1:C:436:MET:HA	1:C:436:MET:CE	2.48	0.43
1:E:308:LYS:HG3	1:E:309:SER:N	2.33	0.43
1:E:465:ASN:HD22	1:E:467:CYS:H	1.65	0.43
1:F:282:ASP:HB3	1:F:313:VAL:CG2	2.45	0.43
1:H:236:LYS:HD2	1:H:237:GLU:N	2.33	0.43
1:C:560:MET:HE2	1:C:563:LEU:HD23	2.01	0.43
1:E:254:THR:HG22	1:E:258:ILE:HB	1.99	0.43
1:A:430:HIS:HB2	1:A:523:ASN:ND2	2.27	0.43
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.87	0.43
1:B:308:LYS:HG3	1:B:309:SER:N	2.32	0.43
1:C:432:ASP:OD2	1:C:460:ARG:HD3	2.18	0.43
1:D:501:GLN:HE21	1:D:509:PRO:CB	2.28	0.43
1:F:513:LEU:CG	1:F:514:LYS:H	2.30	0.43
1:H:265:PRO:HB2	1:H:268:MET:HB2	1.99	0.43
1:A:238:ASP:O	1:A:372:PRO:HD2	2.18	0.43
1:A:282:ASP:HB3	1:A:313:VAL:CG2	2.47	0.43
1:A:547:GLN:HA	1:A:547:GLN:OE1	2.18	0.43
1:C:465:ASN:ND2	1:C:465:ASN:C	2.69	0.43
1:F:512:LYS:HB3	1:F:513:LEU:H	1.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:902:DTT:H42	2:G:902:DTT:H11	1.81	0.43
1:H:432:ASP:O	1:H:436:MET:HB2	2.18	0.43
1:D:549:VAL:O	1:D:553:CYS:HB2	2.19	0.43
1:A:281:LYS:HE2	1:A:418:ASP:OD1	2.19	0.43
1:A:564:MET:O	1:A:568:SER:HB2	2.18	0.43
1:C:465:ASN:HD22	1:C:466:GLY:N	2.15	0.43
1:D:471:LEU:HD23	1:D:493:HIS:CD2	2.54	0.43
1:D:569:ARG:O	1:D:573:LYS:HB2	2.19	0.43
1:E:332:PRO:HB2	1:E:333:VAL:H	1.62	0.43
1:G:384:LEU:HD12	1:G:384:LEU:H	1.83	0.43
1:A:548:GLU:CA	1:A:551:ARG:HB3	2.38	0.43
1:C:258:ILE:HD12	1:C:264:TYR:HB2	2.00	0.43
1:C:391:PHE:HB3	1:C:407:ALA:HB3	2.00	0.43
1:C:479:VAL:HG11	1:C:538:VAL:HG22	2.00	0.43
1:D:281:LYS:NZ	1:D:314:MET:HG3	2.34	0.43
1:H:480:ASN:HB3	1:H:483:SER:OG	2.19	0.43
1:A:258:ILE:HD12	1:A:264:TYR:HB2	2.01	0.43
1:A:362:THR:CG2	1:B:451:GLY:HA3	2.48	0.43
1:A:395:HIS:NE2	1:A:489:VAL:HB	2.34	0.43
1:B:446:LYS:C	1:B:448:GLN:H	2.22	0.43
1:C:382:GLU:OE1	1:C:387:LYS:HE2	2.18	0.43
1:C:395:HIS:CE1	1:C:440:TYR:OH	2.72	0.43
1:D:384:LEU:HB3	1:D:494:ARG:HH22	1.81	0.43
1:E:544:THR:HA	1:E:547:GLN:HG2	1.99	0.43
1:F:473:THR:OG1	1:F:493:HIS:CD2	2.70	0.43
1:H:259:THR:O	1:H:263:GLY:HA2	2.18	0.43
1:A:248:ASP:OD1	1:A:250:ILE:HG12	2.18	0.43
1:C:247:HIS:CE1	1:D:540:ARG:HD2	2.53	0.43
1:E:546:LYS:C	1:E:548:GLU:H	2.22	0.43
1:A:398:THR:HA	1:A:531:VAL:HG23	2.01	0.43
1:D:435:VAL:O	1:D:438:GLU:HG2	2.19	0.43
1:D:448:GLN:NE2	1:D:539:SER:HB3	2.23	0.43
1:E:291:THR:O	1:E:294:ILE:HG22	2.18	0.43
1:F:528:GLU:HA	1:F:531:VAL:HG12	2.00	0.43
1:A:522:ARG:O	1:A:526:ILE:HG12	2.18	0.42
1:B:316:ARG:HB3	1:B:335:TYR:CE1	2.54	0.42
1:B:512:LYS:HB3	1:B:513:LEU:H	1.49	0.42
1:C:248:ASP:OD1	1:C:250:ILE:HG12	2.19	0.42
1:C:457:LYS:HD3	1:C:457:LYS:N	2.05	0.42
1:E:365:LEU:HD23	1:F:559:PHE:CE2	2.54	0.42
1:E:374:LYS:NZ	1:H:537:THR:HG21	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:ASP:O	1:E:408:ALA:HB3	2.20	0.42
1:E:479:VAL:HG11	1:E:538:VAL:HG22	2.01	0.42
1:E:551:ARG:HH21	1:E:552:ARG:HB3	1.84	0.42
1:G:258:ILE:HD13	1:G:264:TYR:HB2	2.01	0.42
1:G:458:PRO:HA	1:G:471:LEU:O	2.19	0.42
1:A:419:LEU:HD12	1:A:419:LEU:HA	1.89	0.42
1:B:391:PHE:CD2	1:B:408:ALA:HB2	2.54	0.42
1:F:444:MET:CE	1:F:486:LEU:HD22	2.48	0.42
1:H:287:ALA:O	1:H:290:ILE:HD13	2.19	0.42
1:H:384:LEU:HD21	1:H:494:ARG:CZ	2.49	0.42
1:H:444:MET:HE1	1:H:486:LEU:HB2	1.99	0.42
1:H:528:GLU:O	1:H:532:LYS:HB2	2.19	0.42
1:D:430:HIS:CE1	1:D:431:GLU:HG3	2.54	0.42
1:E:564:MET:O	1:E:568:SER:HB2	2.19	0.42
1:H:528:GLU:HA	1:H:531:VAL:HG12	2.01	0.42
1:C:460:ARG:HG3	1:C:470:LEU:CD2	2.50	0.42
1:H:264:TYR:HE2	1:H:316:ARG:O	2.03	0.42
1:H:312:CYS:SG	1:H:373:ILE:HD11	2.59	0.42
1:A:547:GLN:C	1:A:549:VAL:H	2.22	0.42
1:B:265:PRO:O	1:B:268:MET:N	2.52	0.42
1:D:391:PHE:CE2	1:D:493:HIS:HB2	2.54	0.42
1:G:469:VAL:HG23	1:G:471:LEU:HD13	2.01	0.42
1:H:340:LEU:N	1:H:340:LEU:HD12	2.34	0.42
1:H:419:LEU:HD12	1:H:419:LEU:HA	1.75	0.42
1:A:435:VAL:O	1:A:438:GLU:HG2	2.19	0.42
1:A:447:GLY:O	1:A:540:ARG:NH2	2.52	0.42
1:A:533:ARG:O	1:A:536:GLU:HB2	2.20	0.42
1:C:340:LEU:N	1:C:340:LEU:HD12	2.35	0.42
1:C:414:TYR:CG	1:C:419:LEU:HD13	2.55	0.42
1:C:479:VAL:HG11	1:C:538:VAL:CG2	2.50	0.42
1:D:312:CYS:HB3	1:D:415:LEU:HD13	2.01	0.42
1:A:546:LYS:C	1:A:548:GLU:H	2.23	0.42
1:D:264:TYR:HA	1:D:265:PRO:HD3	1.93	0.42
1:D:470:LEU:O	1:D:496:PHE:N	2.51	0.42
1:D:248:ASP:OD1	1:D:250:ILE:HG12	2.19	0.42
1:D:404:VAL:CG2	1:D:416:PRO:HA	2.44	0.42
1:D:528:GLU:O	1:D:532:LYS:HB2	2.20	0.42
1:E:376:SER:OG	1:E:410:SER:HB3	2.20	0.42
1:G:546:LYS:C	1:G:548:GLU:H	2.23	0.42
1:H:412:LEU:O	1:H:463:ILE:HB	2.20	0.42
1:H:471:LEU:HD12	1:H:495:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:294:ILE:HA	1:E:295:PRO:HD2	1.63	0.42
1:E:386:GLN:C	1:E:388:SER:H	2.23	0.42
1:E:454:PHE:CE1	1:E:475:TRP:HB2	2.55	0.42
1:H:264:TYR:HA	1:H:265:PRO:HD3	1.90	0.42
1:F:431:GLU:HB2	1:F:460:ARG:HH22	1.84	0.42
1:G:463:ILE:HG12	1:G:467:CYS:O	2.20	0.42
1:G:547:GLN:OE1	1:G:547:GLN:HA	2.19	0.42
1:A:272:ARG:CG	1:A:272:ARG:NH1	2.76	0.41
1:A:412:LEU:O	1:A:463:ILE:HB	2.20	0.41
2:C:903:DTT:H42	2:C:903:DTT:H11	1.69	0.41
1:F:433:LEU:HD12	1:F:523:ASN:ND2	2.35	0.41
1:H:519:ALA:O	1:H:523:ASN:HB2	2.19	0.41
1:C:439:THR:O	1:C:442:THR:HB	2.21	0.41
1:E:347:ALA:HB2	1:E:363:ASN:HD22	1.85	0.41
1:E:517:GLU:HG3	1:E:518:GLU:N	2.26	0.41
1:A:262:LEU:HD22	1:A:317:ARG:HA	2.01	0.41
1:B:351:ALA:O	1:B:352:ARG:CB	2.67	0.41
1:E:391:PHE:CE2	1:E:493:HIS:HB2	2.56	0.41
1:E:433:LEU:HD23	1:E:433:LEU:HA	1.83	0.41
1:F:513:LEU:CG	1:F:514:LYS:N	2.84	0.41
1:G:559:PHE:CZ	1:H:348:PRO:HD3	2.54	0.41
1:H:395:HIS:CD2	1:H:399:GLY:HA2	2.55	0.41
1:F:395:HIS:CD2	1:F:399:GLY:HA2	2.55	0.41
1:F:416:PRO:HD3	2:F:900:DTT:S1	2.61	0.41
1:G:348:PRO:HB2	1:G:349:GLU:H	1.62	0.41
1:G:503:ASN:ND2	1:G:506:GLU:HB3	2.34	0.41
1:G:515:ILE:O	1:G:519:ALA:HB3	2.20	0.41
1:G:544:THR:HG23	1:G:547:GLN:HB2	2.02	0.41
1:H:517:GLU:CG	1:H:518:GLU:H	2.32	0.41
1:A:544:THR:HG23	1:A:547:GLN:HB2	2.01	0.41
1:C:236:LYS:HD2	1:C:236:LYS:C	2.41	0.41
1:C:512:LYS:HB3	1:C:513:LEU:H	1.53	0.41
1:C:513:LEU:CG	1:C:514:LYS:N	2.79	0.41
1:D:384:LEU:HD22	1:D:494:ARG:HH12	1.83	0.41
1:F:265:PRO:O	1:F:267:ASP:N	2.53	0.41
1:G:551:ARG:HH21	1:G:552:ARG:HB3	1.84	0.41
1:H:442:THR:O	1:H:446:LYS:HG2	2.20	0.41
1:H:514:LYS:HG3	1:H:515:ILE:H	1.85	0.41
1:A:317:ARG:HE	1:A:336:GLU:CD	2.23	0.41
1:A:342:LEU:HD22	1:A:368:ILE:HG12	2.01	0.41
1:D:388:SER:HA	1:D:389:PRO:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:444:MET:HE1	1:F:486:LEU:HD22	2.02	0.41
1:G:262:LEU:HD23	1:G:262:LEU:HA	1.92	0.41
1:G:316:ARG:HD2	1:G:335:TYR:OH	2.20	0.41
1:H:351:ALA:O	1:H:352:ARG:CB	2.66	0.41
1:H:521:SER:O	1:H:524:THR:HG22	2.21	0.41
1:A:277:PHE:O	1:A:315:LEU:HA	2.21	0.41
1:A:517:GLU:HG3	1:A:518:GLU:N	2.26	0.41
1:B:272:ARG:HG2	1:B:272:ARG:NH1	2.34	0.41
1:B:473:THR:OG1	1:B:493:HIS:CD2	2.71	0.41
1:D:512:LYS:HD3	1:D:512:LYS:HA	1.85	0.41
1:E:384:LEU:HD12	1:E:384:LEU:H	1.85	0.41
1:H:289:GLN:HG3	1:H:311:PHE:CD2	2.56	0.41
1:H:533:ARG:CG	1:H:533:ARG:NH2	2.84	0.41
1:A:367:VAL:HG21	1:B:563:LEU:CD2	2.51	0.41
1:C:473:THR:HG23	1:C:493:HIS:CD2	2.55	0.41
1:G:522:ARG:HH21	1:G:525:ARG:HD2	1.85	0.41
1:A:448:GLN:HG3	1:A:539:SER:O	2.21	0.41
1:A:473:THR:OG1	1:A:493:HIS:HD2	2.03	0.41
1:C:473:THR:OG1	1:C:493:HIS:CD2	2.73	0.41
1:C:518:GLU:O	1:C:522:ARG:HB3	2.20	0.41
1:D:267:ASP:HB2	1:D:270:LEU:HD12	2.03	0.41
1:D:294:ILE:HD12	1:D:295:PRO:HD2	2.03	0.41
1:D:521:SER:HA	1:D:524:THR:HG22	2.02	0.41
1:H:254:THR:HG21	1:H:258:ILE:HG13	2.03	0.41
1:C:354:ASP:HB2	1:C:355:ASN:H	1.75	0.41
1:D:319:ARG:HH11	1:D:333:VAL:N	2.19	0.41
1:D:463:ILE:HG13	1:D:465:ASN:ND2	2.36	0.41
1:H:342:LEU:CD2	1:H:368:ILE:HG12	2.51	0.41
1:C:559:PHE:CE2	1:D:365:LEU:HD23	2.56	0.40
1:D:311:PHE:CD2	1:D:311:PHE:N	2.90	0.40
1:C:433:LEU:HD12	1:C:523:ASN:HD22	1.86	0.40
1:C:460:ARG:HA	1:C:469:VAL:O	2.20	0.40
1:D:347:ALA:HA	1:D:348:PRO:HD3	1.98	0.40
1:E:395:HIS:CE1	1:E:440:TYR:OH	2.57	0.40
1:A:443:VAL:HG22	1:A:454:PHE:HE1	1.87	0.40
1:A:528:GLU:O	1:A:532:LYS:HB2	2.20	0.40
1:F:262:LEU:HB3	1:F:264:TYR:HD2	1.87	0.40
1:A:512:LYS:HD3	1:A:512:LYS:HA	1.88	0.40
1:A:540:ARG:HD2	1:B:247:HIS:CE1	2.57	0.40
1:A:569:ARG:O	1:A:573:LYS:HB2	2.22	0.40
1:E:550:SER:HA	1:E:553:CYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:CYS:HB3	1:G:415:LEU:HD22	2.03	0.40
1:A:397:ALA:HB2	1:A:486:LEU:O	2.22	0.40
1:B:282:ASP:HB3	1:B:313:VAL:HG23	2.01	0.40
1:B:501:GLN:OE1	2:B:903:DTT:S4	2.79	0.40
1:C:413:GLY:HA3	1:C:464:GLN:HB3	2.02	0.40
1:E:344:PHE:HB3	1:E:364:MET:HE3	2.04	0.40
1:E:530:ILE:O	1:E:534:LEU:HB2	2.21	0.40
1:F:290:ILE:HG22	1:F:342:LEU:CD1	2.51	0.40
1:H:444:MET:CE	1:H:486:LEU:HD22	2.50	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	298/339 (88%)	265 (89%)	23 (8%)	10 (3%)	3	12
1	B	294/339 (87%)	261 (89%)	25 (8%)	8 (3%)	5	16
1	C	294/339 (87%)	264 (90%)	24 (8%)	6 (2%)	7	23
1	D	298/339 (88%)	269 (90%)	19 (6%)	10 (3%)	3	12
1	E	299/339 (88%)	267 (89%)	21 (7%)	11 (4%)	3	11
1	F	294/339 (87%)	262 (89%)	25 (8%)	7 (2%)	6	19
1	G	298/339 (88%)	266 (89%)	23 (8%)	9 (3%)	4	14
1	H	294/339 (87%)	259 (88%)	29 (10%)	6 (2%)	7	23
All	All	2369/2712 (87%)	2113 (89%)	189 (8%)	67 (3%)	5	16

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	513	LEU
1	A	516	SER
1	A	517	GLU
1	B	266	ARG
1	B	352	ARG
1	B	546	LYS
1	C	266	ARG
1	C	352	ARG
1	D	266	ARG
1	D	384	LEU
1	D	513	LEU
1	D	547	GLN
1	E	266	ARG
1	E	295	PRO
1	E	513	LEU
1	E	516	SER
1	E	517	GLU
1	F	266	ARG
1	F	352	ARG
1	G	266	ARG
1	G	516	SER
1	G	517	GLU
1	H	266	ARG
1	H	352	ARG
1	A	348	PRO
1	A	545	VAL
1	A	547	GLN
1	C	546	LYS
1	D	516	SER
1	E	547	GLN
1	F	546	LYS
1	G	348	PRO
1	G	349	GLU
1	H	515	ILE
1	B	512	LYS
1	B	515	ILE
1	B	518	GLU
1	D	238	ASP
1	D	348	PRO
1	F	353	PRO
1	G	295	PRO
1	G	513	LEU

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Mol	Chain	Res	Type
1	H	546	LYS
1	A	238	ASP
1	A	295	PRO
1	B	238	ASP
1	C	512	LYS
1	D	349	GLU
1	E	349	GLU
1	F	512	LYS
1	F	515	ILE
1	G	238	ASP
1	H	512	LYS
1	A	454	PHE
1	C	515	ILE
1	E	348	PRO
1	E	508	ALA
1	H	458	PRO
1	B	545	VAL
1	D	295	PRO
1	E	238	ASP
1	G	508	ALA
1	C	353	PRO
1	F	545	VAL
1	D	508	ALA
1	E	545	VAL

### 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%)	242 (89%)	31 (11%)	5 15
1	B	269/298 (90%)	235 (87%)	34 (13%)	4 11
1	C	269/298 (90%)	231 (86%)	38 (14%)	3 9
1	D	273/298 (92%)	241 (88%)	32 (12%)	5 14
1	E	274/298 (92%)	241 (88%)	33 (12%)	5 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	269/298 (90%)	237 (88%)	32 (12%)	5	13
1	G	273/298 (92%)	245 (90%)	28 (10%)	7	19
1	H	269/298 (90%)	228 (85%)	41 (15%)	3	7
All	All	2169/2384 (91%)	1900 (88%)	269 (12%)	4	12

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LYS
1	A	251	VAL
1	A	252	LEU
1	A	258	ILE
1	A	268	MET
1	A	290	ILE
1	A	291	THR
1	A	294	ILE
1	A	296	ILE
1	A	313	VAL
1	A	348	PRO
1	A	350	GLU
1	A	371	THR
1	A	406	SER
1	A	417	GLN
1	A	419	LEU
1	A	436	MET
1	A	448	GLN
1	A	457	LYS
1	A	465	ASN
1	A	471	LEU
1	A	487	GLU
1	A	490	VAL
1	A	495	VAL
1	A	506	GLU
1	A	511	CYS
1	A	513	LEU
1	A	514	LYS
1	A	528	GLU
1	A	560	MET
1	A	564	MET
1	B	236	LYS
1	B	251	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	252	LEU
1	B	258	ILE
1	B	268	MET
1	B	280	LEU
1	B	290	ILE
1	B	310	THR
1	B	313	VAL
1	B	319	ARG
1	B	352	ARG
1	B	354	ASP
1	B	371	THR
1	B	387	LYS
1	B	417	GLN
1	B	419	LEU
1	B	436	MET
1	B	448	GLN
1	B	457	LYS
1	B	464	GLN
1	B	465	ASN
1	B	485	LYS
1	B	490	VAL
1	B	518	GLU
1	B	524	THR
1	B	528	GLU
1	B	533	ARG
1	B	534	LEU
1	B	537	THR
1	B	538	VAL
1	B	545	VAL
1	B	553	CYS
1	B	560	MET
1	B	565	ASP
1	C	236	LYS
1	C	244	ILE
1	C	251	VAL
1	C	258	ILE
1	C	267	ASP
1	C	272	ARG
1	C	280	LEU
1	C	281	LYS
1	C	290	ILE
1	C	309	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	310	THR
1	C	313	VAL
1	C	317	ARG
1	C	319	ARG
1	C	350	GLU
1	C	352	ARG
1	C	354	ASP
1	C	371	THR
1	C	384	LEU
1	C	387	LYS
1	C	417	GLN
1	C	419	LEU
1	C	436	MET
1	C	448	GLN
1	C	457	LYS
1	C	465	ASN
1	C	472	GLU
1	C	485	LYS
1	C	490	VAL
1	C	524	THR
1	C	528	GLU
1	C	533	ARG
1	C	537	THR
1	C	538	VAL
1	C	545	VAL
1	C	549	VAL
1	C	553	CYS
1	C	560	MET
1	D	236	LYS
1	D	251	VAL
1	D	254	THR
1	D	258	ILE
1	D	260	ASP
1	D	290	ILE
1	D	296	ILE
1	D	317	ARG
1	D	350	GLU
1	D	371	THR
1	D	398	THR
1	D	406	SER
1	D	417	GLN
1	D	419	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	436	MET
1	D	448	GLN
1	D	457	LYS
1	D	458	PRO
1	D	465	ASN
1	D	485	LYS
1	D	490	VAL
1	D	506	GLU
1	D	513	LEU
1	D	514	LYS
1	D	518	GLU
1	D	520	GLN
1	D	528	GLU
1	D	534	LEU
1	D	537	THR
1	D	540	ARG
1	D	564	MET
1	D	574	LEU
1	E	236	LYS
1	E	239	SER
1	E	251	VAL
1	E	252	LEU
1	E	258	ILE
1	E	260	ASP
1	E	290	ILE
1	E	296	ILE
1	E	310	THR
1	E	313	VAL
1	E	319	ARG
1	E	333	VAL
1	E	350	GLU
1	E	371	THR
1	E	395	HIS
1	E	406	SER
1	E	416	PRO
1	E	417	GLN
1	E	419	LEU
1	E	436	MET
1	E	448	GLN
1	E	457	LYS
1	E	465	ASN
1	E	471	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	485	LYS
1	E	490	VAL
1	E	495	VAL
1	E	506	GLU
1	E	513	LEU
1	E	514	LYS
1	E	528	GLU
1	E	534	LEU
1	E	564	MET
1	F	236	LYS
1	F	244	ILE
1	F	251	VAL
1	F	252	LEU
1	F	258	ILE
1	F	280	LEU
1	F	281	LYS
1	F	290	ILE
1	F	313	VAL
1	F	319	ARG
1	F	350	GLU
1	F	352	ARG
1	F	354	ASP
1	F	371	THR
1	F	384	LEU
1	F	387	LYS
1	F	417	GLN
1	F	448	GLN
1	F	457	LYS
1	F	460	ARG
1	F	465	ASN
1	F	485	LYS
1	F	524	THR
1	F	528	GLU
1	F	533	ARG
1	F	534	LEU
1	F	537	THR
1	F	545	VAL
1	F	551	ARG
1	F	553	CYS
1	F	560	MET
1	F	565	ASP
1	G	236	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	252	LEU
1	G	258	ILE
1	G	281	LYS
1	G	290	ILE
1	G	296	ILE
1	G	313	VAL
1	G	350	GLU
1	G	371	THR
1	G	406	SER
1	G	417	GLN
1	G	419	LEU
1	G	435	VAL
1	G	436	MET
1	G	448	GLN
1	G	457	LYS
1	G	465	ASN
1	G	471	LEU
1	G	485	LYS
1	G	506	GLU
1	G	513	LEU
1	G	514	LYS
1	G	524	THR
1	G	528	GLU
1	G	538	VAL
1	G	552	ARG
1	G	560	MET
1	G	564	MET
1	H	236	LYS
1	H	238	ASP
1	H	251	VAL
1	H	252	LEU
1	H	258	ILE
1	H	280	LEU
1	H	290	ILE
1	H	310	THR
1	H	313	VAL
1	H	317	ARG
1	H	319	ARG
1	H	350	GLU
1	H	352	ARG
1	H	354	ASP
1	H	365	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	371	THR
1	H	384	LEU
1	H	387	LYS
1	H	406	SER
1	H	417	GLN
1	H	419	LEU
1	H	436	MET
1	H	448	GLN
1	H	457	LYS
1	H	464	GLN
1	H	465	ASN
1	H	471	LEU
1	H	485	LYS
1	H	490	VAL
1	H	518	GLU
1	H	524	THR
1	H	528	GLU
1	H	533	ARG
1	H	534	LEU
1	H	537	THR
1	H	538	VAL
1	H	545	VAL
1	H	546	LYS
1	H	553	CYS
1	H	560	MET
1	H	565	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	395	HIS
1	A	403	HIS
1	A	417	GLN
1	A	429	HIS
1	A	465	ASN
1	A	493	HIS
1	A	497	GLN
1	A	523	ASN
1	B	395	HIS
1	B	403	HIS
1	B	417	GLN
1	B	429	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	465	ASN
1	B	492	HIS
1	B	493	HIS
1	B	501	GLN
1	B	523	ASN
1	B	547	GLN
1	C	247	HIS
1	C	395	HIS
1	C	403	HIS
1	C	417	GLN
1	C	429	HIS
1	C	464	GLN
1	C	465	ASN
1	C	493	HIS
1	C	501	GLN
1	C	523	ASN
1	D	363	ASN
1	D	395	HIS
1	D	403	HIS
1	D	417	GLN
1	D	429	HIS
1	D	448	GLN
1	D	465	ASN
1	D	493	HIS
1	D	501	GLN
1	D	503	ASN
1	D	523	ASN
1	E	247	HIS
1	E	363	ASN
1	E	395	HIS
1	E	403	HIS
1	E	417	GLN
1	E	429	HIS
1	E	448	GLN
1	E	465	ASN
1	E	493	HIS
1	E	503	ASN
1	E	523	ASN
1	F	395	HIS
1	F	403	HIS
1	F	417	GLN
1	F	429	HIS

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Mol	Chain	Res	Type
1	F	465	ASN
1	F	493	HIS
1	F	501	GLN
1	F	547	GLN
1	G	363	ASN
1	G	395	HIS
1	G	403	HIS
1	G	417	GLN
1	G	429	HIS
1	G	465	ASN
1	G	493	HIS
1	G	503	ASN
1	G	523	ASN
1	H	395	HIS
1	H	417	GLN
1	H	429	HIS
1	H	465	ASN
1	H	493	HIS
1	H	523	ASN
1	H	547	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 monosaccharides 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	C	900	1	7,7,7	0.82	0	4,8,8	0.32	0
2	DTT	H	900	1	7,7,7	0.82	0	4,8,8	0.47	0
2	DTT	H	902	1	7,7,7	1.02	0	4,8,8	0.76	0
2	DTT	G	902	1	7,7,7	0.94	0	4,8,8	0.27	0
2	DTT	D	901	1	7,7,7	1.01	0	4,8,8	0.58	0
2	DTT	F	903	1	7,7,7	1.45	1 (14%)	4,8,8	0.52	0
2	DTT	F	902	1	7,7,7	0.77	0	4,8,8	0.45	0
2	DTT	B	903	1	7,7,7	0.96	0	4,8,8	0.20	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	D	902	1	7,7,7	0.97	0	4,8,8	0.41	0
2	DTT	G	901	1	7,7,7	1.05	0	4,8,8	0.63	0
2	DTT	B	900	1	7,7,7	0.82	0	4,8,8	0.66	0
2	DTT	C	901	1	7,7,7	0.83	0	4,8,8	0.19	0
2	DTT	B	901	1	7,7,7	0.90	0	4,8,8	0.63	0
2	DTT	D	900	1	7,7,7	0.60	0	4,8,8	0.34	0
2	DTT	G	900	1	7,7,7	0.72	0	4,8,8	0.49	0
2	DTT	H	901	1	7,7,7	0.96	0	4,8,8	0.71	0
2	DTT	A	903	1	7,7,7	0.74	0	4,8,8	0.40	0
2	DTT	E	900	1	7,7,7	0.76	0	4,8,8	0.37	0
2	DTT	C	903	1	7,7,7	1.35	1 (14%)	4,8,8	0.77	0
2	DTT	E	901	1	7,7,7	1.09	1 (14%)	4,8,8	0.72	0
2	DTT	F	900	1	7,7,7	0.84	0	4,8,8	0.51	0
2	DTT	C	902	1	7,7,7	0.93	0	4,8,8	0.48	0
2	DTT	A	900	1	7,7,7	0.74	0	4,8,8	0.44	0
2	DTT	A	902	1	7,7,7	0.89	0	4,8,8	0.46	0
2	DTT	B	902	1	7,7,7	0.94	0	4,8,8	0.46	0
2	DTT	F	901	1	7,7,7	0.90	0	4,8,8	0.50	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	C	900	1	-	6/8/8/8	-
2	DTT	H	900	1	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTT	H	902	1	-	4/8/8/8	-
2	DTT	G	902	1	-	3/8/8/8	-
2	DTT	D	901	1	-	6/8/8/8	-
2	DTT	F	903	1	-	2/8/8/8	-
2	DTT	F	902	1	-	6/8/8/8	-
2	DTT	B	903	1	-	1/8/8/8	-
2	DTT	A	901	1	-	7/8/8/8	-
2	DTT	H	903	1	-	2/8/8/8	-
2	DTT	D	902	1	-	5/8/8/8	-
2	DTT	G	901	1	-	7/8/8/8	-
2	DTT	B	900	1	-	6/8/8/8	-
2	DTT	C	901	1	-	6/8/8/8	-
2	DTT	B	901	1	-	6/8/8/8	-
2	DTT	D	900	1	-	4/8/8/8	-
2	DTT	G	900	1	-	3/8/8/8	-
2	DTT	H	901	1	-	5/8/8/8	-
2	DTT	A	903	1	-	4/8/8/8	-
2	DTT	E	900	1	-	2/8/8/8	-
2	DTT	C	903	1	-	6/8/8/8	-
2	DTT	E	901	1	-	6/8/8/8	-
2	DTT	F	900	1	-	5/8/8/8	-
2	DTT	C	902	1	-	6/8/8/8	-
2	DTT	A	900	1	-	5/8/8/8	-
2	DTT	A	902	1	-	3/8/8/8	-
2	DTT	B	902	1	-	4/8/8/8	-
2	DTT	F	901	1	-	5/8/8/8	-

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.

All (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
2	A	901	DTT	C1-C2-C3-C4
2	A	901	DTT	O2-C2-C3-O3
2	A	901	DTT	O2-C2-C3-C4
2	A	901	DTT	C2-C3-C4-S4
2	A	901	DTT	O3-C3-C4-S4
2	A	902	DTT	C2-C3-C4-S4
2	A	902	DTT	O3-C3-C4-S4
2	A	903	DTT	S1-C1-C2-C3
2	A	903	DTT	C2-C3-C4-S4
2	A	903	DTT	O3-C3-C4-S4
2	B	900	DTT	S1-C1-C2-O2
2	B	900	DTT	S1-C1-C2-C3
2	B	900	DTT	C1-C2-C3-O3
2	B	900	DTT	C1-C2-C3-C4
2	B	900	DTT	O2-C2-C3-O3
2	B	900	DTT	O2-C2-C3-C4
2	B	901	DTT	S1-C1-C2-O2
2	B	901	DTT	S1-C1-C2-C3
2	B	901	DTT	C1-C2-C3-O3
2	B	901	DTT	C1-C2-C3-C4
2	B	901	DTT	O2-C2-C3-O3
2	B	901	DTT	O2-C2-C3-C4
2	B	902	DTT	C1-C2-C3-O3
2	B	902	DTT	O2-C2-C3-O3
2	B	902	DTT	O2-C2-C3-C4
2	B	903	DTT	O3-C3-C4-S4
2	C	900	DTT	S1-C1-C2-O2
2	C	900	DTT	S1-C1-C2-C3
2	C	900	DTT	C1-C2-C3-O3
2	C	900	DTT	C1-C2-C3-C4
2	C	900	DTT	O2-C2-C3-O3
2	C	900	DTT	O2-C2-C3-C4
2	C	901	DTT	S1-C1-C2-O2
2	C	901	DTT	S1-C1-C2-C3
2	C	901	DTT	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	C	901	DTT	C1-C2-C3-C4
2	C	901	DTT	O2-C2-C3-O3
2	C	901	DTT	O2-C2-C3-C4
2	C	902	DTT	S1-C1-C2-O2
2	C	902	DTT	S1-C1-C2-C3
2	C	902	DTT	C1-C2-C3-O3
2	C	902	DTT	C1-C2-C3-C4
2	C	902	DTT	O2-C2-C3-O3
2	C	902	DTT	O2-C2-C3-C4
2	C	903	DTT	S1-C1-C2-O2
2	C	903	DTT	S1-C1-C2-C3
2	C	903	DTT	C1-C2-C3-C4
2	C	903	DTT	O2-C2-C3-O3
2	C	903	DTT	C2-C3-C4-S4
2	C	903	DTT	O3-C3-C4-S4
2	D	900	DTT	C1-C2-C3-O3
2	D	900	DTT	C1-C2-C3-C4
2	D	900	DTT	O2-C2-C3-O3
2	D	900	DTT	O2-C2-C3-C4
2	D	901	DTT	C1-C2-C3-O3
2	D	901	DTT	C1-C2-C3-C4
2	D	901	DTT	O2-C2-C3-O3
2	D	901	DTT	O2-C2-C3-C4
2	D	901	DTT	C2-C3-C4-S4
2	D	901	DTT	O3-C3-C4-S4
2	D	902	DTT	C1-C2-C3-O3
2	D	902	DTT	C1-C2-C3-C4
2	D	902	DTT	O2-C2-C3-O3
2	D	902	DTT	C2-C3-C4-S4
2	D	902	DTT	O3-C3-C4-S4
2	E	900	DTT	C1-C2-C3-C4
2	E	901	DTT	S1-C1-C2-O2
2	E	901	DTT	C1-C2-C3-O3
2	E	901	DTT	O2-C2-C3-O3
2	E	901	DTT	O2-C2-C3-C4
2	E	901	DTT	C2-C3-C4-S4
2	E	901	DTT	O3-C3-C4-S4
2	F	900	DTT	S1-C1-C2-O2
2	F	900	DTT	S1-C1-C2-C3
2	F	900	DTT	C1-C2-C3-O3
2	F	900	DTT	O2-C2-C3-O3
2	F	900	DTT	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	F	901	DTT	S1-C1-C2-O2
2	F	901	DTT	S1-C1-C2-C3
2	F	901	DTT	C1-C2-C3-C4
2	F	902	DTT	S1-C1-C2-O2
2	F	902	DTT	S1-C1-C2-C3
2	F	902	DTT	C1-C2-C3-O3
2	F	902	DTT	C1-C2-C3-C4
2	F	902	DTT	O2-C2-C3-O3
2	F	902	DTT	O2-C2-C3-C4
2	F	903	DTT	C2-C3-C4-S4
2	F	903	DTT	O3-C3-C4-S4
2	G	900	DTT	C1-C2-C3-C4
2	G	900	DTT	O2-C2-C3-C4
2	G	901	DTT	S1-C1-C2-O2
2	G	901	DTT	C1-C2-C3-O3
2	G	901	DTT	C1-C2-C3-C4
2	G	901	DTT	O2-C2-C3-O3
2	G	901	DTT	O2-C2-C3-C4
2	G	901	DTT	C2-C3-C4-S4
2	G	901	DTT	O3-C3-C4-S4
2	G	902	DTT	C1-C2-C3-C4
2	G	902	DTT	O2-C2-C3-O3
2	G	902	DTT	O3-C3-C4-S4
2	H	900	DTT	S1-C1-C2-O2
2	H	900	DTT	S1-C1-C2-C3
2	H	900	DTT	C1-C2-C3-O3
2	H	900	DTT	C1-C2-C3-C4
2	H	900	DTT	O2-C2-C3-O3
2	H	900	DTT	O2-C2-C3-C4
2	H	901	DTT	S1-C1-C2-O2
2	H	901	DTT	S1-C1-C2-C3
2	H	901	DTT	C1-C2-C3-C4
2	H	901	DTT	O2-C2-C3-C4
2	H	902	DTT	S1-C1-C2-O2
2	H	902	DTT	C1-C2-C3-O3
2	H	902	DTT	O2-C2-C3-O3
2	H	902	DTT	O2-C2-C3-C4
2	H	903	DTT	S1-C1-C2-O2
2	H	903	DTT	S1-C1-C2-C3
2	A	900	DTT	O2-C2-C3-O3
2	A	902	DTT	O2-C2-C3-O3
2	A	900	DTT	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	E	900	DTT	O2-C2-C3-C4
2	F	901	DTT	O2-C2-C3-C4
2	H	901	DTT	C1-C2-C3-O3
2	A	903	DTT	S1-C1-C2-O2
2	B	902	DTT	S1-C1-C2-O2
2	G	900	DTT	C1-C2-C3-O3
2	F	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	C	900	DTT	2	0
2	G	902	DTT	2	0
2	F	903	DTT	4	0
2	B	903	DTT	1	0
2	H	903	DTT	4	0
2	D	902	DTT	1	0
2	B	900	DTT	1	0
2	C	901	DTT	1	0
2	B	901	DTT	1	0
2	D	900	DTT	1	0
2	H	901	DTT	1	0
2	A	903	DTT	1	0
2	C	903	DTT	4	0
2	F	900	DTT	4	0
2	A	900	DTT	1	0
2	A	902	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	306/339 (90%)	0.03	13 (4%) 36 31	31, 56, 125, 134	0
1	B	302/339 (89%)	-0.04	9 (2%) 50 45	32, 58, 115, 130	0
1	C	302/339 (89%)	0.11	13 (4%) 35 30	29, 60, 126, 142	0
1	D	306/339 (90%)	0.17	22 (7%) 15 11	31, 63, 130, 147	0
1	E	307/339 (90%)	0.18	23 (7%) 14 10	28, 56, 128, 146	0
1	F	302/339 (89%)	0.09	14 (4%) 32 27	32, 64, 127, 139	0
1	G	306/339 (90%)	0.08	18 (5%) 22 17	30, 58, 128, 136	0
1	H	302/339 (89%)	0.23	14 (4%) 32 27	43, 78, 120, 144	0
All	All	2433/2712 (89%)	0.11	126 (5%) 27 22	28, 62, 126, 147	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	356	TYR	8.7
1	C	353	PRO	8.0
1	E	574	LEU	7.7
1	E	572	LEU	7.5
1	D	350	GLU	7.4
1	D	574	LEU	6.8
1	C	356	TYR	6.7
1	C	307	ALA	6.3
1	H	355	ASN	6.0
1	E	350	GLU	6.0
1	E	573	LYS	5.9
1	D	573	LYS	5.9
1	E	571	ASP	5.9
1	A	571	ASP	5.8
1	B	353	PRO	5.7
1	E	349	GLU	5.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	H	353	PRO	5.6
1	A	572	LEU	5.5
1	G	350	GLU	5.5
1	D	349	GLU	5.3
1	F	356	TYR	5.2
1	B	356	TYR	5.2
1	C	354	ASP	5.1
1	D	571	ASP	5.0
1	G	571	ASP	4.9
1	F	353	PRO	4.8
1	H	319	ARG	4.7
1	D	572	LEU	4.7
1	E	518	GLU	4.6
1	C	547	GLN	4.5
1	G	387	LYS	4.5
1	E	307	ALA	4.4
1	D	514	LYS	4.4
1	G	518	GLU	4.3
1	G	572	LEU	4.3
1	C	513	LEU	4.2
1	A	236	LYS	4.2
1	B	355	ASN	4.1
1	F	307	ALA	4.1
1	E	544	THR	4.0
1	D	544	THR	3.9
1	A	350	GLU	3.9
1	E	513	LEU	3.9
1	G	544	THR	3.8
1	G	509	PRO	3.8
1	D	547	GLN	3.8
1	E	547	GLN	3.8
1	H	351	ALA	3.7
1	F	549	VAL	3.7
1	A	544	THR	3.7
1	F	550	SER	3.6
1	H	354	ASP	3.5
1	D	542	SER	3.5
1	F	354	ASP	3.4
1	A	546	LYS	3.3
1	G	574	LEU	3.3
1	D	550	SER	3.3
1	C	352	ARG	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	547	GLN	3.2
1	C	236	LYS	3.1
1	E	508	ALA	3.1
1	F	236	LYS	3.1
1	D	508	ALA	3.1
1	F	546	LYS	3.1
1	G	361	GLY	3.1
1	E	361	GLY	3.0
1	D	361	GLY	2.9
1	H	543	GLU	2.9
1	D	307	ALA	2.9
1	C	355	ASN	2.9
1	B	236	LYS	2.9
1	A	509	PRO	2.7
1	E	348	PRO	2.7
1	E	542	SER	2.7
1	D	570	ALA	2.7
1	G	349	GLU	2.7
1	A	387	LYS	2.7
1	A	542	SER	2.6
1	E	546	LYS	2.6
1	G	309	SER	2.6
1	E	386	GLN	2.6
1	H	549	VAL	2.6
1	G	542	SER	2.6
1	G	508	ALA	2.6
1	G	573	LYS	2.6
1	E	387	LYS	2.5
1	A	518	GLU	2.5
1	H	387	LYS	2.5
1	H	518	GLU	2.5
1	F	513	LEU	2.5
1	H	544	THR	2.5
1	A	574	LEU	2.5
1	F	352	ARG	2.4
1	C	549	VAL	2.4
1	B	319	ARG	2.4
1	F	553	CYS	2.4
1	D	236	LYS	2.4
1	D	515	ILE	2.4
1	E	309	SER	2.3
1	F	319	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	570	ALA	2.3
1	A	543	GLU	2.3
1	B	350	GLU	2.3
1	C	319	ARG	2.3
1	F	355	ASN	2.3
1	D	549	VAL	2.3
1	A	349	GLU	2.3
1	B	543	GLU	2.3
1	G	548	GLU	2.2
1	H	389	PRO	2.2
1	G	546	LYS	2.2
1	B	348	PRO	2.2
1	C	545	VAL	2.2
1	H	333	VAL	2.2
1	C	543	GLU	2.2
1	D	377	TYR	2.1
1	G	513	LEU	2.1
1	G	545	VAL	2.1
1	B	513	LEU	2.1
1	H	545	VAL	2.1
1	D	543	GLU	2.1
1	D	295	PRO	2.1
1	E	543	GLU	2.1
1	E	550	SER	2.0
1	E	549	VAL	2.0
1	D	513	LEU	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 monosaccharides 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, 95<sup>th</sup> 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	A	902	8/8	0.40	0.69	136,140,143,146	0
2	DTT	D	901	8/8	0.58	0.50	108,115,119,120	0
2	DTT	H	900	8/8	0.64	0.25	104,105,109,112	0
2	DTT	D	902	8/8	0.66	0.66	135,141,142,143	0
2	DTT	H	901	8/8	0.66	0.27	112,117,120,121	0
2	DTT	A	901	8/8	0.71	0.38	99,107,111,111	0
2	DTT	F	902	8/8	0.71	0.38	119,120,121,124	0
2	DTT	G	902	8/8	0.72	0.59	130,131,132,132	0
2	DTT	G	901	8/8	0.73	0.42	103,106,109,110	0
2	DTT	E	901	8/8	0.74	0.25	104,112,115,116	0
2	DTT	H	903	8/8	0.74	0.23	135,139,141,142	0
2	DTT	A	903	8/8	0.75	0.41	124,136,139,142	0
2	DTT	H	902	8/8	0.77	0.30	96,100,104,110	0
2	DTT	B	900	8/8	0.78	0.27	80,83,89,97	0
2	DTT	F	901	8/8	0.78	0.27	94,98,103,105	0
2	DTT	C	903	8/8	0.78	0.49	125,137,140,143	0
2	DTT	F	903	8/8	0.79	0.28	129,136,138,140	0
2	DTT	C	901	8/8	0.80	0.30	96,104,110,114	0
2	DTT	B	903	8/8	0.80	0.54	125,135,139,141	0
2	DTT	B	901	8/8	0.82	0.25	85,90,97,100	0
2	DTT	E	900	8/8	0.82	0.21	74,77,82,87	0
2	DTT	D	900	8/8	0.83	0.22	71,75,81,88	0
2	DTT	F	900	8/8	0.85	0.21	82,89,95,102	0
2	DTT	C	900	8/8	0.85	0.17	77,83,90,99	0
2	DTT	B	902	8/8	0.86	0.35	98,106,112,117	0
2	DTT	C	902	8/8	0.86	0.23	102,107,110,115	0
2	DTT	G	900	8/8	0.86	0.28	71,74,85,91	0
2	DTT	A	900	8/8	0.90	0.23	74,77,84,89	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.