



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:43 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

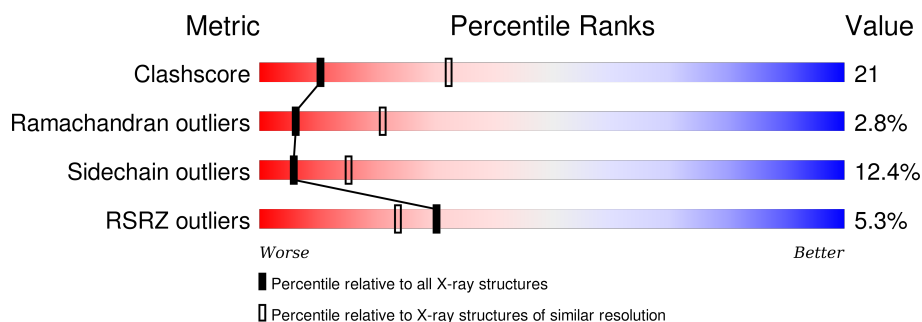
1 Overall quality at a glance

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	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>4%</div> <div> <div>47%</div> <div>36%</div> <div>7%</div> <div>10%</div> </div> </div>
1	B	339	<div> <div>3%</div> <div> <div>53%</div> <div>30%</div> <div>6%</div> <div>11%</div> </div> </div>
1	C	339	<div> <div>4%</div> <div> <div>51%</div> <div>29%</div> <div>8%</div> <div>11%</div> </div> </div>
1	D	339	<div> <div>6%</div> <div> <div>48%</div> <div>36%</div> <div>6%</div> <div>10%</div> </div> </div>
1	E	339	<div> <div>6%</div> <div> <div>47%</div> <div>36%</div> <div>7%</div> <div>9%</div> </div> </div>
1	F	339	<div> <div>4%</div> <div> <div>52%</div> <div>31%</div> <div>6%</div> <div>11%</div> </div> </div>
1	G	339	<div> <div>6%</div> <div> <div>57%</div> <div>29%</div> <div>5%</div> <div>10%</div> </div> </div>

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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	B	900	-	-	-	X
2	DTT	B	901	-	-	-	X
2	DTT	B	902	-	-	-	X
2	DTT	B	903	-	-	-	X
2	DTT	C	901	-	-	-	X
2	DTT	C	903	-	-	X	X
2	DTT	D	902	-	-	-	X
2	DTT	F	900	-	-	X	-
2	DTT	F	901	-	-	-	X
2	DTT	F	903	-	-	X	-
2	DTT	G	900	-	-	-	X
2	DTT	G	902	-	-	-	X
2	DTT	H	901	-	-	-	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
1	A	306	Total	C	N	O	S	0	0	0
			2436	1549	419	450	18			
1	B	302	Total	C	N	O	S	0	0	0
			2410	1530	415	447	18			
1	C	302	Total	C	N	O	S	0	0	0
			2410	1530	415	447	18			
1	D	306	Total	C	N	O	S	0	0	0
			2436	1549	419	450	18			
1	E	307	Total	C	N	O	S	0	0	0
			2443	1554	420	451	18			
1	F	302	Total	C	N	O	S	0	0	0
			2410	1530	415	447	18			
1	G	306	Total	C	N	O	S	0	0	0
			2436	1549	419	450	18			
1	H	302	Total	C	N	O	S	0	0	0
			2410	1530	415	447	18			

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: $\text{C}_4\text{H}_{10}\text{O}_2\text{S}_2$).



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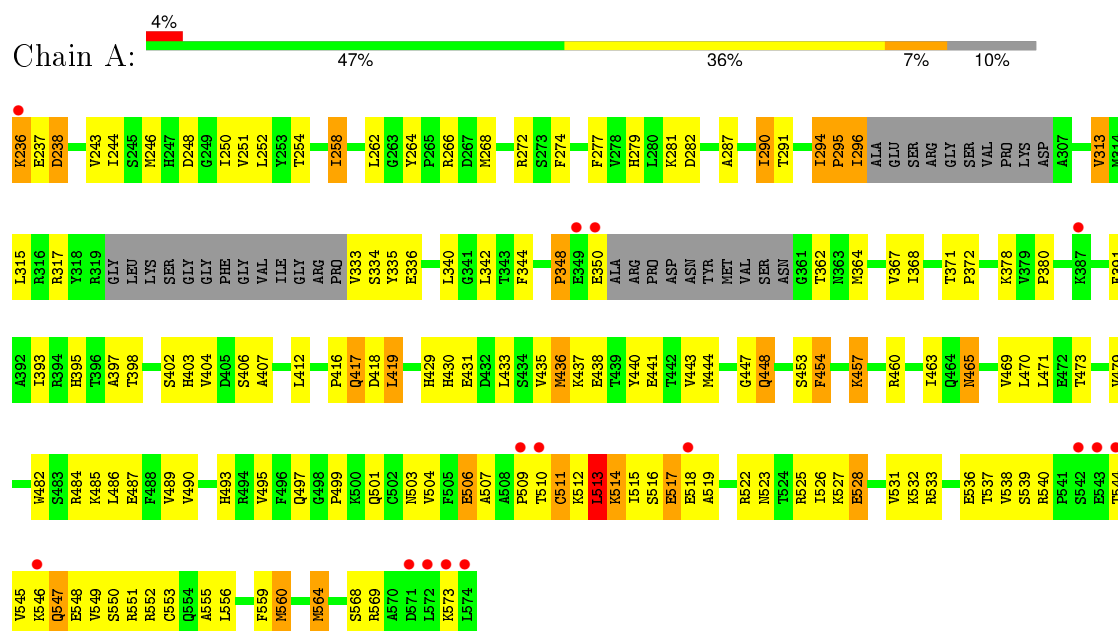
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	33	Total 33	O 33	0	0
3	G	28	Total 28	O 28	0	0
3	H	21	Total 21	O 21	0	0

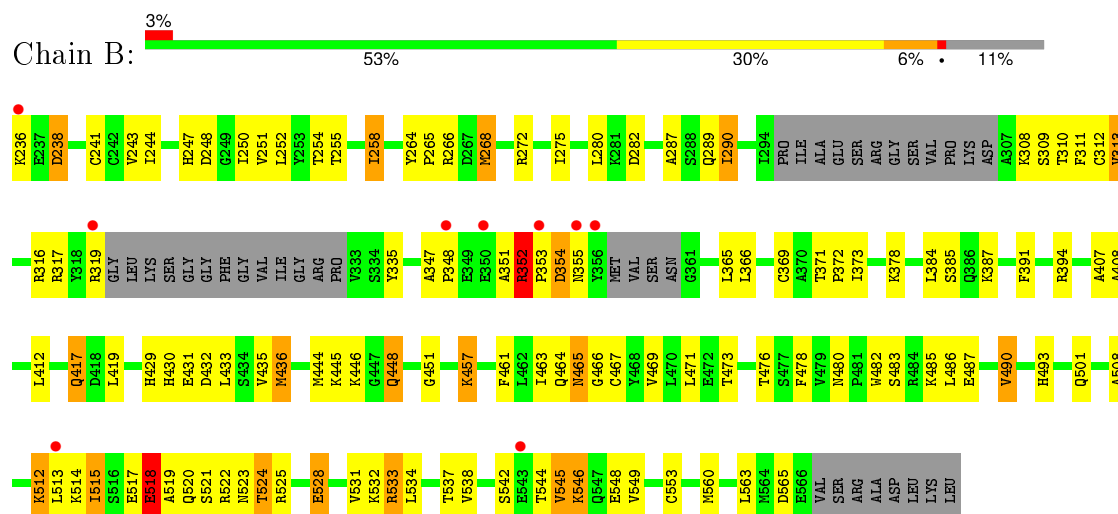
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

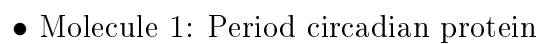
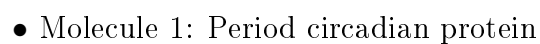
• Molecule 1: Period circadian protein

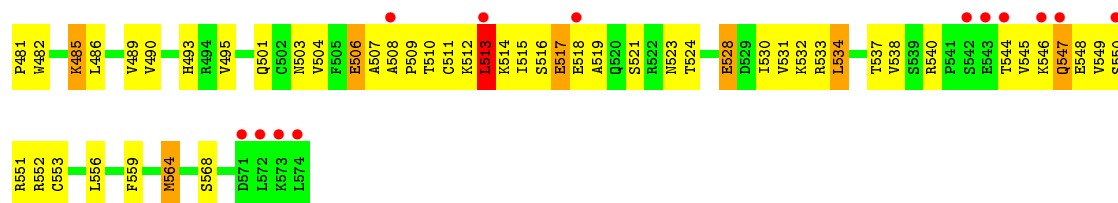


• Molecule 1: Period circadian protein

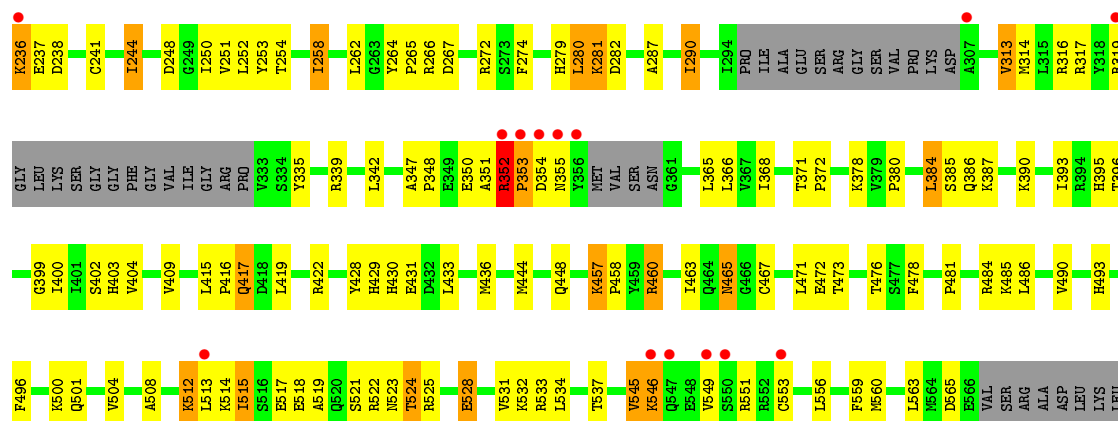


• Molecule 1: Period circadian protein

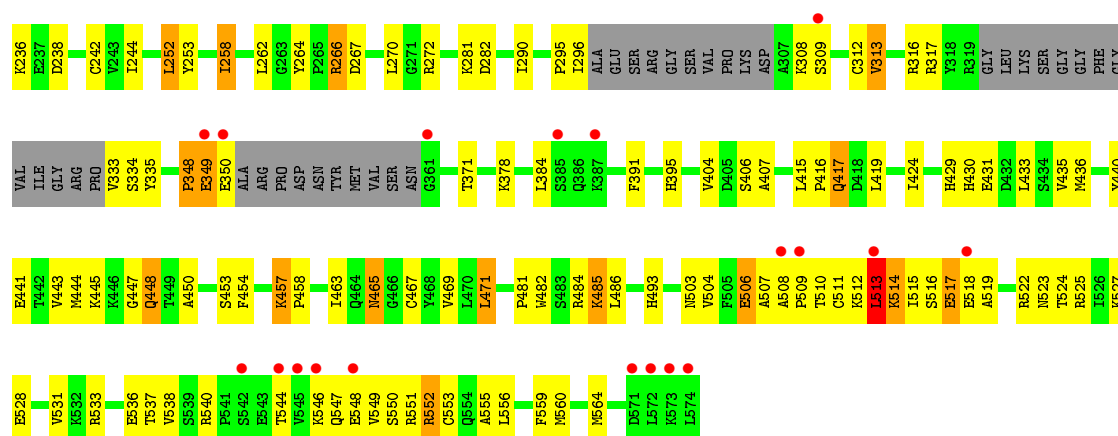




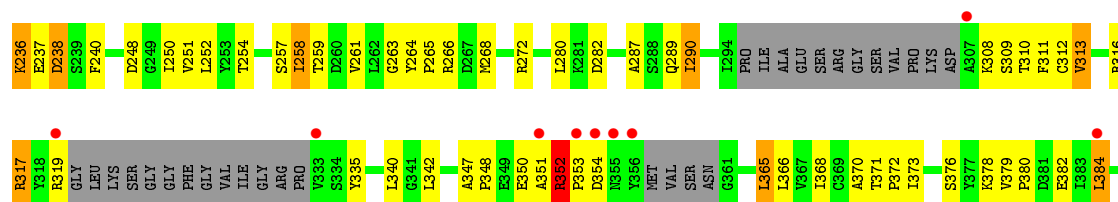
• Molecule 1: Period circadian protein

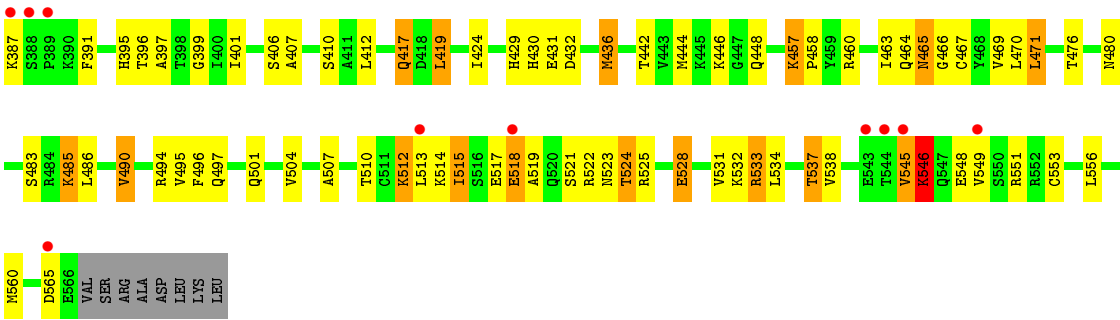


• Molecule 1: Period circadian protein



• Molecule 1: Period circadian protein





4 Data and refinement statistics

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 20.14 – 2.86	Depositor EDS
% Data completeness (in resolution range)	92.4 (20.01-2.85) 86.4 (20.14-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.83Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.239 , 0.289 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	64.1	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.2	EDS
Estimated twinning fraction	0.095 for h,-k,-l 0.069 for -h,k,-l 0.068 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 66028 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19848	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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

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:HD3	1:G:457:LYS:H	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:H42	2:H:903:DTT:S1	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:HH21	1:H:317:ARG:HB3	1.33	0.92
1:F:380:PRO:HB3	2:F:903:DTT:S4	2.11	0.91
1:B:417:GLN:NE2	1:B:417:GLN:H	1.69	0.90
1:H:465:ASN:ND2	1:H:467:CYS:H	1.71	0.89
1:B:417:GLN:HE21	1:B:417:GLN:H	0.92	0.89
1:E:457:LYS:HD3	1:E:457:LYS:H	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:D:457:LYS:H	1:D:457:LYS:HD3	1.39	0.87
1:C:272:ARG:HG2	1:C:272:ARG:HH11	1.36	0.87
1:C:417:GLN:HE21	1:C:417:GLN:H	1.23	0.86
1:A:272:ARG:HH11	1:A:272:ARG:HG2	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:HH11	1:F:272:ARG:HG2	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:H:347:ALA:HB2	1:H:365:LEU:HD13	1.57	0.84
1:G:417:GLN:H	1:G:417:GLN:HE21	1.26	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:B:429:HIS:HD2	1:B:431:GLU:H	1.30	0.79
1:A:417:GLN:HE21	1:A:417:GLN: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:H	1:B:457:LYS:HD3	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:H:501:GLN:OE1	2:H:903:DTT:S4	2.45	0.74
1:G:308:LYS:HG3	1:G:309:SER:H	1.51	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:F:517:GLU:HG3	1:F:518:GLU:H	1.53	0.74
1:C:515:ILE:O	1:C:519:ALA:HB3	1.88	0.74
1:G:465:ASN:O	1:G:509:PRO:HD2	1.86	0.74
1:A:391:PHE:HB3	1:A:407:ALA:HB3	1.68	0.74
1:D:437:LYS:O	1:D:441:GLU:HG3	1.88	0.73
1:B:317:ARG:HH21	1:B:317:ARG:HB3	1.53	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:H:465:ASN:HD22	1:H:467:CYS:H	1.36	0.73
1:E:512:LYS:O	1:E:513:LEU:HB3	1.88	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:E:507:ALA:O	1:E:509:PRO:HD3	1.89	0.72
1:A:512:LYS:O	1:A:513:LEU:HB3	1.90	0.72
1:H:485:LYS:HE2	1:H:537:THR:HB	1.70	0.72
1:E:272:ARG:HH11	1:E:272:ARG:HG2	1.54	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:G:417:GLN:H	1:G:417:GLN:NE2	1.88	0.71
1:E:548:GLU:HA	1:E:551:ARG:HB3	1.72	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:H:533:ARG:HH21	1:H:533:ARG:HG2	1.59	0.68
1:G:514:LYS:HD2	1:G:514:LYS:O	1.93	0.68
1:C:517:GLU:HG3	1:C:518:GLU:H	1.59	0.68
1:A:465:ASN:O	1:A:509:PRO:HD2	1.93	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:H:429:HIS:HD2	1:H:431:GLU:H	1.42	0.67
1:B:528:GLU:HA	1:B:531:VAL:HG12	1.76	0.67
1:G:430:HIS:HB2	1:G:523:ASN:HD21	1.59	0.67
1:D:317:ARG:HB3	1:D:317:ARG:HH21	1.60	0.67
1:G:513:LEU:HD12	1:G:514:LYS:N	2.09	0.67
1:H:352:ARG:H	1:H:353:PRO:CD	2.07	0.66
1:C:243:VAL:HG23	1:D:564:MET:SD	2.35	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:H:317:ARG:NH2	1:H:317:ARG:HB3	2.08	0.66
1:E:457:LYS:HD3	1:E:457:LYS:N	2.10	0.66
1:D:282:ASP:HB3	1:D:313:VAL:HG22	1.76	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:HD22	1:B:465:ASN:C	1.98	0.66
1:E:258:ILE:CD1	1:E:264:TYR:HB2	2.26	0.65
1:F:352:ARG:H	1:F:353:PRO:HD2	1.62	0.65
1:A:254:THR:CG2	1:A:258:ILE:HG13	2.26	0.65
1:G:317:ARG:HH21	1:G:317:ARG:HB3	1.60	0.65
1:A:463:ILE:HD12	1:A:504:VAL:HG23	1.77	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:C:465:ASN:C	1:C:465:ASN:HD22	2.00	0.65
1:D:457:LYS:N	1:D:457:LYS:HD3	2.11	0.65
1:A:404:VAL:HG21	1:A:416:PRO:HA	1.77	0.65
1:D:272:ARG:HH11	1:D:272:ARG:HG2	1.61	0.65
1:C:444:MET:HE1	1:C:486:LEU:HD22	1.79	0.65
1:C:429:HIS:HD2	1:C:431:GLU:H	1.44	0.64
1:C:352:ARG:N	1:C:353:PRO:CD	2.59	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:E:515:ILE:HG23	1:E:519:ALA:HB2	1.78	0.64
1:G:507:ALA:O	1:G:509:PRO:HD3	1.97	0.64
1:F:428:TYR:CD1	1:F:436:MET:HG2	2.33	0.64
1:C:514:LYS:HG3	1:C:515:ILE:H	1.62	0.64
1:A:282:ASP:HB3	1:A:313:VAL:HG23	1.79	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:CD	1:G:457:LYS:H	2.06	0.63
1:E:457:LYS:CD	1:E:457:LYS:H	2.10	0.63
1:H:457:LYS:H	1:H:457:LYS:CD	2.05	0.63
1:H:351:ALA:O	1:H:352:ARG:HB2	1.97	0.63
1:B:521:SER:HB3	1:B:525:ARG:NH1	2.14	0.63
1:D:384:LEU:CD2	1:D:496:PHE:HA	2.28	0.63
1:C:451:GLY:HA3	1:D:362:THR:HG22	1.80	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:H:352:ARG:N	1:H:353:PRO:CD	2.62	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: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:NH2	1:F:317:ARG:HB3	2.14	0.62
1:D:457:LYS:CD	1:D:457:LYS:H	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:C:457:LYS:H	1:C:457:LYS:CD	2.01	0.62
1:B:238:ASP:O	1:B:372:PRO:HD2	2.00	0.62
1:G:550:SER:HB2	1:G:556:LEU:HD22	1.81	0.62
1:E:465:ASN:HD22	1:E:465:ASN:C	2.03	0.61
1:F:457:LYS:H	1:F:457:LYS:CD	2.07	0.61
1:G:417:GLN:N	1:G:417:GLN:HE21	1.95	0.61
1:H:257:SER:O	1:H:261:VAL:HG23	2.00	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:B:272:ARG:HG2	1:B:272:ARG:HH11	1.66	0.61
1:H:521:SER:HB3	1:H:525:ARG:NH1	2.12	0.61
1:D:514:LYS:HE2	1:D:519:ALA:HB3	1.82	0.61
1:A:479:VAL:HG11	1:A:538:VAL:HG21	1.83	0.61
1:C:412:LEU:O	1:C:463:ILE:HB	2.00	0.61
1:B:546:LYS:O	1:B:549:VAL:HG12	2.00	0.61
1:C:502:CYS:N	2:C:903:DTT:S1	2.71	0.61
1:H:436:MET:HA	1:H:436:MET:CE	2.31	0.61
1:G:317:ARG:NH2	1:G:317:ARG:HB3	2.14	0.61
1:G:559:PHE:CE2	1:H:348:PRO:HD3	2.36	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:E:509:PRO:O	1:E:510:THR:HG22	2.02	0.60
2:H:903:DTT:S1	2:H:903:DTT:C4	2.81	0.60
1:E:485:LYS:HE2	1:E:537:THR:HB	1.83	0.60
1:F:546:LYS:O	1:F:549:VAL:HG12	2.01	0.60
1:F:347:ALA:HB2	1:F:365:LEU:HD13	1.83	0.60
1:E:308:LYS:HG3	1:E:309:SER:H	1.66	0.60
1:E:465:ASN:O	1:E:509:PRO:HD2	2.00	0.60
1:H:248:ASP:OD1	1:H:250:ILE:HG12	2.02	0.60
1:E:417:GLN:H	1:E:417:GLN:HE21	1.50	0.60
1:D:465:ASN:ND2	1:D:467:CYS:H	1.99	0.60
1:H:417:GLN:NE2	1:H:417:GLN:H	1.96	0.60
1:G:262:LEU:HD22	1:G:317:ARG:HA	1.82	0.60
1:B:287:ALA:O	1:B:290:ILE:HD13	2.02	0.60
1:A:548:GLU:HA	1:A:551:ARG:CB	2.32	0.60
1:G:378:LYS:N	1:G:378:LYS:HD2	2.17	0.60
1:C:282:ASP:HB3	1:C:313:VAL:CG2	2.32	0.60
1:G:484:ARG:HH11	1:G:484:ARG:HG2	1.67	0.60
2:F:903:DTT:C4	2:F:903:DTT:S1	2.89	0.59
1:G:444:MET:CE	1:G:486:LEU:HD22	2.32	0.59
1:D:316:ARG:HB3	1:D:335:TYR:CE1	2.37	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:G:457:LYS:N	1:G:457:LYS:HD3	2.07	0.59
1:E:437:LYS:O	1:E:441:GLU:HG3	2.03	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:NH2	1:B:317:ARG:HB3	2.17	0.59
1:C:469:VAL:HG23	1:C:471:LEU:HD13	1.85	0.59
1:B:391:PHE:HB3	1:B:407:ALA:HB3	1.85	0.59
1:H:444:MET:HE1	1:H:486:LEU:HD22	1.84	0.59
1:H:465:ASN:C	1:H:465:ASN:HD22	2.06	0.59
1:A:272:ARG:CG	1:A:272:ARG:HH11	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:C:465:ASN:ND2	1:C:467:CYS:HB2	2.11	0.58
1:A:551:ARG:HH21	1:A:552:ARG:HB3	1.68	0.58
1:A:429:HIS:HD2	1:A:431:GLU:H	1.50	0.58
1:E:503:ASN:HD22	1:E:506:GLU:HB3	1.69	0.58
1:F:521:SER:HB3	1:F:525:ARG:NH1	2.09	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:A:453:SER:O	1:A:454:PHE:HB3	2.02	0.58
1:G:465:ASN:HD22	1:G:465:ASN:C	2.07	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: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: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:533:ARG:HH21	1:C:533:ARG:HG2	1.68	0.57
1:D:236:LYS:HD2	1:D:237:GLU:N	2.20	0.57
1:C:348:PRO:HD3	1:D:559:PHE:CE2	2.40	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:513:LEU:CG	1:C:514:LYS:H	2.17	0.57
1:C:241:CYS:HB2	1:D:564:MET:HG3	1.85	0.57
1:D:517:GLU:HG3	1:D:518:GLU:H	1.70	0.57
1:D:258:ILE:O	1:D:258:ILE:HD13	2.05	0.56
1:E:296:ILE:HD11	1:F:478:PHE:HB2	1.86	0.56
1:H:465:ASN:HD22	1:H:466:GLY:N	2.04	0.56
1:D:384:LEU:HB3	1:D:494:ARG:NH2	2.20	0.56
1:A:509:PRO:O	1:A:510:THR:HG22	2.06	0.56
1:F:317:ARG:HB3	1:F:317:ARG:HH21	1.70	0.56
1:C:282:ASP:HB3	1:C:313:VAL:HG22	1.87	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:D:253:TYR:HE1	1:D:266:ARG:HH12	1.54	0.56
1:H:395:HIS:HD2	1:H:396:THR:O	1.87	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:559:PHE:CE2	1:B:348:PRO:HD3	2.39	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:518:GLU:O	1:D:522:ARG:HB3	2.05	0.56
1:F:465:ASN:C	1:F:465:ASN:HD22	2.09	0.56
1:D:378:LYS:O	1:D:502:CYS:SG	2.64	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:H12	2:C:901:DTT:S4	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:B:465:ASN:HD22	1:B:467:CYS:H	1.51	0.55
1:A:507:ALA:O	1:A:509:PRO:HD3	2.06	0.55
1:F:378:LYS:HD2	1:F:378:LYS:N	2.21	0.55
1:H:532:LYS:HD3	1:H:532:LYS:O	2.06	0.55
1:F:384:LEU:HD12	1:F:496:PHE:HA	1.88	0.55
1:A:294:ILE:HG13	1:A:295:PRO:HD2	1.88	0.55
2:B:901:DTT:S4	2:B:901:DTT:S1	3.00	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:H:465:ASN:HA	1:H:507:ALA:HA	1.89	0.55
1:G:548:GLU:HA	1:G:551:ARG:CB	2.36	0.55
1:A:417:GLN:NE2	1:A:417:GLN:H	2.02	0.55
1:E:348:PRO:HD3	1:E:365:LEU:HD22	1.88	0.55
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:A:550:SER:HB2	1:A:556:LEU:HD22	1.89	0.54
1:B:532:LYS:HD3	1:B:532:LYS:O	2.07	0.54
1:G:465:ASN:ND2	1:G:467:CYS:H	2.05	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:H:513:LEU:HG	1:H:514:LYS:N	2.22	0.54
1:H:401:ILE:HD13	1:H:419:LEU:HG	1.89	0.54
1:D:509:PRO:O	1:D:510:THR:HG22	2.07	0.54
1:B:430:HIS:HB2	1:B:523:ASN:ND2	2.22	0.54
1:B:384:LEU:HD23	1:B:385:SER:N	2.22	0.54
1:B:378:LYS:HD2	1:B:378:LYS:N	2.21	0.54
1:C:517:GLU:O	1:C:521:SER:HB2	2.08	0.54
1:B:412:LEU:O	1:B:463:ILE:HB	2.08	0.54
1:G:522:ARG:HA	1:G:522:ARG:HE	1.73	0.54
1:D:439:THR:O	1:D:443:VAL:HG23	2.08	0.54
1:F:517:GLU:O	1:F:521:SER:HB2	2.08	0.54
1:A:503:ASN:ND2	1:A:506:GLU:HB3	2.22	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:HG2	1:G:272:ARG:HH11	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:NH1	1:A:272:ARG:HG2	2.19	0.53
1:E:384:LEU:HD12	1:E:384:LEU:N	2.23	0.53
1:E:548:GLU:HA	1:E:551:ARG:CB	2.39	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: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: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:F:528:GLU:O	1:F:532:LYS:HB2	2.08	0.53
1:D:526:ILE:O	1:D:530:ILE:HG13	2.09	0.53
1:B:412:LEU:HD13	1:B:461:PHE:CE1	2.44	0.53
1:H:397:ALA:HB2	1:H:486:LEU:O	2.09	0.52
1:D:281:LYS:HE2	1:D:418:ASP:OD1	2.10	0.52
1:H:548:GLU:HG3	1:H:551:ARG:NH2	2.23	0.52
1:F:429:HIS:HD2	1:F:431:GLU:H	1.54	0.52
1:F:352:ARG:H	1:F:353:PRO:HD3	1.73	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:A:236:LYS:HD2	1:A:237:GLU:N	2.24	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:433:LEU:HD12	1:C:523:ASN:ND2	2.25	0.52
1:C:251:VAL:HG13	1:C:269:TRP:O	2.09	0.52
1:D:258:ILE:CD1	1:D:264:TYR:HB2	2.36	0.52
1:B:501:GLN:NE2	1:B:508:ALA:HB1	2.19	0.52
1:B:469:VAL:HG23	1:B:471:LEU:HD13	1.92	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: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:308:LYS:HG3	1:D:309:SER:H	1.75	0.52
1:A:484:ARG:HE	1:A:540:ARG:HB2	1.73	0.52
1:H:352:ARG:N	1:H:353:PRO:HD2	2.15	0.52
1:E:253:TYR:HE1	1:E:266:ARG:NH1	2.08	0.52
1:G:544:THR:HA	1:G:547:GLN:HG2	1.91	0.52
1:D:503:ASN:ND2	1:D:506:GLU:HB3	2.25	0.52
1:G:441:GLU:HG2	1:G:533:ARG:CD	2.40	0.52
1:C:417:GLN:NE2	1:C:417:GLN:H	2.02	0.52
1:B:457:LYS:CD	1:B:457:LYS:H	2.20	0.52
1:H:460:ARG:HA	1:H:469:VAL:O	2.10	0.52
1:F:513:LEU:HG	1:F:514:LYS:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:SER:HB2	1:E:371:THR:HB	1.91	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
1:E:236:LYS:HD2	1:E:237:GLU:N	2.25	0.51
2:D:900:DTT:H12	2:D:900:DTT:S4	2.50	0.51
1:E:481:PRO:HG2	1:E:482:TRP:CE3	2.45	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: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:F:339:ARG:HH21	2:F:900:DTT:H11	1.76	0.51
1:D:444:MET:HE2	1:D:444:MET:HA	1.93	0.51
1:C:473:THR:OG1	1:C:493:HIS:HD2	1.93	0.51
1:D:463:ILE:HG12	1:D:467:CYS:O	2.10	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:259:THR:O	1:D:263:GLY:HA2	2.11	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:N	1:E:378:LYS:HD2	2.26	0.51
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:F:238:ASP:O	1:F:372:PRO:HD2	2.11	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: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:A:522:ARG:HH21	1:A:525:ARG:HD2	1.77	0.50
1:A:362:THR:HG22	1:B:451:GLY:HA3	1.94	0.50
1:F:352:ARG:N	1:F:353:PRO:CD	2.64	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:B:515:ILE:O	1:B:519:ALA:HB3	2.12	0.50
1:F:518:GLU:O	1:F:522:ARG:HB3	2.12	0.50
1:B:465:ASN:HD21	1:B:467:CYS:HB2	1.76	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:C:379:VAL:HB	1:C:380:PRO:HD2	1.92	0.50
1:G:509:PRO:O	1:G:510:THR:HG22	2.12	0.50
1:C:476:THR:OG1	1:C:490:VAL:HG13	2.12	0.50
1:E:479:VAL:HG11	1:E:538:VAL:HG21	1.94	0.50
1:E:447:GLY:O	1:E:540:ARG:NH2	2.44	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:H:546:LYS:O	1:H:549:VAL:HG12	2.12	0.50
1:C:482:TRP:HB3	1:D:275:ILE:HD13	1.93	0.50
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:564:MET:CG	1:B:241:CYS:HB2	2.42	0.49
1:E:272:ARG:NH1	1:E:272:ARG:HG2	2.27	0.49
1:A:313:VAL:HG12	1:A:340:LEU:CD1	2.42	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:A:378:LYS:N	1:A:378:LYS:HD2	2.26	0.49
1:C:339:ARG:HH21	2:C:900:DTT:H11	1.77	0.49
1:G:533:ARG:O	1:G:536:GLU:HB2	2.12	0.49
1:F:473:THR:OG1	1:F:493:HIS:HD2	1.95	0.49
1:A:499:PRO:HG2	1:A:501:GLN:O	2.12	0.49
1:D:465:ASN:HD22	1:D:466:GLY:N	2.10	0.49
1:D:383:ILE:CG2	1:D:384:LEU:N	2.75	0.49
1:D:484:ARG:HE	1:D:540:ARG:HB2	1.78	0.49
1:D:469:VAL:HG23	1:D:471:LEU:HD13	1.94	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:H:517:GLU:HG3	1:H:518:GLU:H	1.77	0.49
1:G:267:ASP:HB2	1:G:270:LEU:HG	1.93	0.49
1:E:511:CYS:O	1:E:512:LYS:HG2	2.13	0.49
1:E:290:ILE:HG22	1:E:342:LEU:HD11	1.95	0.49
1:C:347:ALA:HB2	1:C:365:LEU:HD13	1.95	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:258:ILE:O	1:C:258:ILE:HD13	2.12	0.49
1:F:417:GLN:H	1:F:417:GLN:NE2	2.04	0.48
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: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:H:469:VAL:HG23	1:H:471:LEU:HD13	1.95	0.48
1:E:528:GLU:O	1:E:532:LYS:HB2	2.13	0.48
1:E:342:LEU:CD2	1:E:368:ILE:HG12	2.43	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:F:272:ARG:HG2	1:F:272:ARG:NH1	2.19	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:D:465:ASN:HB2	1:D:509:PRO:HD2	1.94	0.48
1:G:444:MET:HE2	1:G:444:MET:HA	1.95	0.48
1:E:392:ALA:H	1:E:405:ASP:HB2	1.79	0.48
1:C:417:GLN:HE21	1:C:417:GLN:N	2.02	0.48
1:E:510:THR:HG23	1:E:511:CYS:N	2.28	0.48
1:C:378:LYS:HD3	1:C:387:LYS:HZ1	1.79	0.48
1:H:342:LEU:HD22	1:H:366:LEU:HD11	1.94	0.48
1:F:458:PRO:HG3	1:F:472:GLU:HB3	1.94	0.48
1:D:311:PHE:HE2	1:D:342:LEU:HG	1.78	0.48
1:H:465:ASN:HD21	1:H:467:CYS:H	1.59	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:C:307:ALA:HB1	1:D:571:ASP:OD1	2.14	0.48
1:H:518:GLU:O	1:H:522:ARG:HB3	2.14	0.48
1:F:417:GLN:N	1:F:417:GLN:HE21	2.05	0.48
1:A:344:PHE:HB3	1:A:364:MET:HE1	1.94	0.48
1:G:447:GLY:O	1:G:540:ARG:NH2	2.46	0.48
1:B:444:MET:HE3	1:B:486:LEU:HB2	1.95	0.48
1:F:521:SER:O	1:F:524:THR:HG22	2.14	0.48
1:E:461:PHE:CB	1:E:471:LEU:HD22	2.43	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:C:522:ARG:HE	1:C:522:ARG:HA	1.79	0.47
1:F:522:ARG:HE	1:F:522:ARG:HA	1.79	0.47
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:D:550:SER:HA	1:D:553:CYS:HB2	1.96	0.47
1:C:380:PRO:HB3	2:C:903:DTT:O2	2.14	0.47
1:G:481:PRO:HG2	1:G:482:TRP:CE3	2.50	0.47
1:E:281:LYS:HE2	1:E:418:ASP:OD1	2.13	0.47
1:A:436:MET:HA	1:A:436:MET:CE	2.42	0.47
1:E:501:GLN:HE21	1:E:509:PRO:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:MET:CE	1:E:486:LEU:HD22	2.44	0.47
1:F:279:HIS:ND1	1:F:280:LEU:N	2.61	0.47
1:F:342:LEU:HD22	1:F:368:ILE:HG12	1.96	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:H:384:LEU:HD21	1:H:494:ARG:NH1	2.29	0.47
1:C:380:PRO:HB3	2:C:903:DTT:HO2	1.78	0.47
1:B:244:ILE:HB	1:B:366:LEU:HB3	1.97	0.47
1:G:511:CYS:O	1:G:512:LYS:HG2	2.14	0.47
1:G:444:MET:HE3	1:G:486:LEU:HD22	1.96	0.47
1:E:481:PRO:HG2	1:E:482:TRP:CD2	2.50	0.47
1:B:436:MET:CE	1:B:436:MET:HA	2.44	0.47
1:H:501:GLN:NE2	1:H:510:THR:HG21	2.29	0.47
1:E:253:TYR:HB2	1:F:556:LEU:HD13	1.96	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: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:C:342:LEU:HD13	1:C:366:LEU:HD11	1.96	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
1:C:238:ASP:O	1:C:372:PRO:HD2	2.15	0.47
2:H:901:DTT:H12	2:H:901:DTT:H42	1.55	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:C:315:LEU:HD12	1:C:338:PHE:CD2	2.50	0.47
1:E:258:ILE:O	1:E:258:ILE:HD13	2.14	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:E:294:ILE:O	1:E:294:ILE:HG23	2.15	0.46
1:E:547:GLN:HA	1:E:547:GLN:OE1	2.15	0.46
1:A:417:GLN:HE21	1:A:417:GLN:N	2.05	0.46
1:H:463:ILE:HD12	1:H:504:VAL:HG12	1.97	0.46
1:G:333:VAL:HG22	1:G:334:SER:N	2.30	0.46
1:G:395:HIS:CE1	1:G:424:ILE:HG21	2.51	0.46
1:B:480:ASN:HB3	1:B:483:SER:OG	2.15	0.46
1:A:522:ARG:HA	1:A:522:ARG:HE	1.81	0.46
1:H:424:ILE:HD11	3:H:142:HOH:O	2.15	0.46
1:C:542:SER:C	1:C:544:THR:H	2.18	0.46
1:D:465:ASN:HB2	1:D:509:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:THR:HB	1:E:367:VAL:HB	1.97	0.46
1:D:383:ILE:HG22	1:D:384:LEU:N	2.29	0.46
1:B:528:GLU:O	1:B:532:LYS:HB2	2.15	0.46
1:F:244:ILE:HD12	1:F:274:PHE:HB2	1.98	0.46
1:F:457:LYS:HD3	1:F:457:LYS:N	2.11	0.46
1:F:351:ALA:O	1:F:352:ARG:HB2	2.13	0.46
1:B:525:ARG:HH11	1:B:525:ARG:HG3	1.80	0.46
1:F:258:ILE:HD13	1:F:258:ILE:O	2.16	0.46
1:E:435:VAL:O	1:E:438:GLU:HG2	2.16	0.46
2:A:900:DTT:H12	2:A:900:DTT:S4	2.55	0.46
1:F:253:TYR:HD2	1:F:254:THR:N	2.13	0.46
1:H:417:GLN:HE21	1:H:417:GLN:N	2.02	0.46
1:G:450:ALA:HB2	1:G:540:ARG:NH1	2.31	0.46
1:H:272:ARG:HH11	1:H:272:ARG:HG2	1.81	0.46
1:A:402:SER:OG	1:A:403:HIS:HD2	1.99	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: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:B:476:THR:OG1	1:B:490:VAL:HG13	2.16	0.46
1:C:517:GLU:HG3	1:C:518:GLU:N	2.27	0.46
1:H:465:ASN:HD21	1:H:467:CYS:HB2	1.80	0.46
1:D:547:GLN:C	1:D:549:VAL:H	2.19	0.46
1:A:497:GLN:NE2	1:F:386:GLN:HB2	2.31	0.46
1:F:352:ARG:HA	1:F:352:ARG:HD2	1.75	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: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:G:550:SER:HB2	1:G:556:LEU:CD2	2.46	0.45
1:C:279:HIS:ND1	1:C:280:LEU:N	2.64	0.45
1:H:429:HIS:CD2	1:H:431:GLU:H	2.27	0.45
1:C:241:CYS:SG	1:C:369:CYS:SG	3.01	0.45
1:H:513:LEU:HG	1:H:514:LYS:H	1.81	0.45
1:D:521:SER:O	1:D:524:THR:HG22	2.17	0.45
1:D:473:THR:HB	1:D:475:TRP:NE1	2.31	0.45
1:H:522:ARG:HE	1:H:522:ARG:HA	1.82	0.45
1:E:237:GLU:O	1:E:238:ASP:C	2.55	0.45
1:D:555:ALA:HB2	2:D:902:DTT:H2	1.99	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:HA	1:B:522:ARG:HE	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:G:512:LYS:O	1:G:513:LEU:HB3	2.15	0.45
1:F:409:VAL:HG21	2:F:900:DTT:S1	2.57	0.45
1:A:244:ILE:HD12	1:A:274:PHE:HB2	1.99	0.45
1:G:391:PHE:HB3	1:G:407:ALA:HB3	1.98	0.45
1:A:279:HIS:HD2	1:A:335:TYR:CD2	2.35	0.45
1:D:515:ILE:CG2	1:D:519:ALA:HB2	2.47	0.45
1:A:513:LEU:HD12	1:A:514:LYS:N	2.32	0.45
1:H:533:ARG:CG	1:H:533:ARG:HH21	2.29	0.45
1:C:444:MET:HE2	1:C:444:MET:HA	1.98	0.45
1:G:429:HIS:HD2	1:G:431:GLU:H	1.64	0.45
1:D:429:HIS:HD2	1:D:431:GLU:H	1.64	0.45
1:D:272:ARG:NH1	1:D:272:ARG:HG2	2.30	0.45
1:B:308:LYS:HG3	1:B:309:SER:H	1.82	0.45
1:E:465:ASN:ND2	1:E:467:CYS:H	2.15	0.45
1:A:395:HIS:CE1	1:A:440:TYR:OH	2.61	0.45
1:G:544:THR:HA	1:G:547:GLN:CG	2.47	0.45
1:F:281:LYS:NZ	1:F:415:LEU:HD12	2.32	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:F:236:LYS:HD2	1:F:237:GLU:N	2.31	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:E:395:HIS:ND1	1:E:424:ILE:HG21	2.31	0.44
1:B:465:ASN:ND2	1:B:465:ASN:C	2.66	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:F:248:ASP:OD1	1:F:250:ILE:HG12	2.18	0.44
1:E:412:LEU:O	1:E:463:ILE:HB	2.17	0.44
1:D:460:ARG:HG3	1:D:470:LEU:CD2	2.47	0.44
1:B:519:ALA:O	1:B:523:ASN:HB2	2.16	0.44
1:F:390:LYS:HA	1:F:493:HIS:O	2.18	0.44
1:G:527:LYS:O	1:G:531:VAL:HG12	2.17	0.44
1:G:471:LEU:HD23	1:G:493:HIS:CD2	2.53	0.44
1:H:485:LYS:HE2	1:H:537:THR:CB	2.44	0.44
1:H:308:LYS:HG3	1:H:309:SER:H	1.82	0.44
1:D:481:PRO:HG2	1:D:482:TRP:CE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:ARG:HB3	1:E:403:HIS:HB2	1.99	0.44
1:A:393:ILE:HG12	1:A:404:VAL:HG12	1.98	0.44
1:E:344:PHE:CE1	1:E:366:LEU:HD13	2.52	0.44
1:D:548:GLU:HA	1:D:551:ARG:CB	2.48	0.44
1:A:290:ILE:HG13	1:B:482:TRP:HZ3	1.83	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:N	1:G:384:LEU:HD12	2.32	0.44
1:G:513:LEU:HD12	1:G:513:LEU:C	2.38	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:B:289:GLN:HG3	1:B:311:PHE:CD2	2.52	0.44
1:A:482:TRP:HB3	1:B:275:ILE:CD1	2.48	0.44
1:E:395:HIS:CD2	1:E:395:HIS:C	2.91	0.44
1:D:404:VAL:HG23	1:D:416:PRO:HG3	2.00	0.44
1:C:545:VAL:HG12	1:C:546:LYS:H	1.82	0.44
1:C:367:VAL:HG21	1:D:563:LEU:HG	2.00	0.44
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.77	0.44
1:B:525:ARG:NH1	1:B:525:ARG:HG3	2.32	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:E:308:LYS:HG3	1:E:309:SER:N	2.33	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:H:236:LYS:HD2	1:H:237:GLU:N	2.33	0.43
1:A:527:LYS:O	1:A:531:VAL:HG12	2.18	0.43
1:C:436:MET:HA	1:C:436:MET:CE	2.48	0.43
1:E:254:THR:HG22	1:E:258:ILE:HB	1.99	0.43
1:C:560:MET:HE2	1:C:563:LEU:HD23	2.01	0.43
1:D:501:GLN:HE21	1:D:509:PRO:CB	2.28	0.43
1:A:430:HIS:HB2	1:A:523:ASN:ND2	2.27	0.43
1:C:432:ASP:OD2	1:C:460:ARG:HD3	2.18	0.43
1:H:265:PRO:HB2	1:H:268:MET:HB2	1.99	0.43
1:F:513:LEU:CG	1:F:514:LYS:H	2.30	0.43
1:B:308:LYS:HG3	1:B:309:SER:N	2.32	0.43
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.87	0.43
1:C:465:ASN:ND2	1:C:465:ASN:C	2.69	0.43
1:A:547:GLN:HA	1:A:547:GLN:OE1	2.18	0.43
1:H:432:ASP:O	1:H:436:MET:HB2	2.18	0.43
1:A:282:ASP:HB3	1:A:313:VAL:CG2	2.47	0.43
2:G:902:DTT:H42	2:G:902:DTT:H11	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:512:LYS:HB3	1:F:513:LEU:H	1.47	0.43
1:A:238:ASP:O	1:A:372:PRO:HD2	2.18	0.43
1:D:549:VAL:O	1:D:553:CYS:HB2	2.19	0.43
1:C:465:ASN:HD22	1:C:466:GLY:N	2.15	0.43
1:A:564:MET:O	1:A:568:SER:HB2	2.18	0.43
1:D:471:LEU:HD23	1:D:493:HIS:CD2	2.54	0.43
1:G:384:LEU:HD12	1:G:384:LEU:H	1.83	0.43
1:D:569:ARG:O	1:D:573:LYS:HB2	2.19	0.43
1:A:281:LYS:HE2	1:A:418:ASP:OD1	2.19	0.43
1:E:332:PRO:HB2	1:E:333:VAL:H	1.62	0.43
1:A:548:GLU:CA	1:A:551:ARG:HB3	2.38	0.43
1:D:281:LYS:NZ	1:D:314:MET:HG3	2.34	0.43
1:C:258:ILE:HD12	1:C:264:TYR:HB2	2.00	0.43
1:C:479:VAL:HG11	1:C:538:VAL:HG22	2.00	0.43
1:C:391:PHE:HB3	1:C:407:ALA:HB3	2.00	0.43
1:H:480:ASN:HB3	1:H:483:SER:OG	2.19	0.43
1:D:384:LEU:HB3	1:D:494:ARG:HH22	1.81	0.43
1:A:395:HIS:NE2	1:A:489:VAL:HB	2.34	0.43
1:A:258:ILE:HD12	1:A:264:TYR:HB2	2.01	0.43
1:C:395:HIS:CE1	1:C:440:TYR:OH	2.72	0.43
1:A:362:THR:CG2	1:B:451:GLY:HA3	2.48	0.43
1:F:473:THR:OG1	1:F:493:HIS:CD2	2.70	0.43
1:C:382:GLU:OE1	1:C:387:LYS:HE2	2.18	0.43
1:E:544:THR:HA	1:E:547:GLN:HG2	1.99	0.43
1:B:446:LYS:C	1:B:448:GLN:H	2.22	0.43
1:H:259:THR:O	1:H:263:GLY:HA2	2.18	0.43
1:E:546:LYS:C	1:E:548:GLU:H	2.22	0.43
1:C:247:HIS:CE1	1:D:540:ARG:HD2	2.53	0.43
1:A:248:ASP:OD1	1:A:250:ILE:HG12	2.18	0.43
1:D:448:GLN:NE2	1:D:539:SER:HB3	2.23	0.43
1:F:528:GLU:HA	1:F:531:VAL:HG12	2.00	0.43
1:E:291:THR:O	1:E:294:ILE:HG22	2.18	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:C:457:LYS:N	1:C:457:LYS:HD3	2.05	0.42
1:E:374:LYS:NZ	1:H:537:THR:HG21	2.34	0.42
1:E:551:ARG:HH21	1:E:552:ARG:HB3	1.84	0.42
1:E:479:VAL:HG11	1:E:538:VAL:HG22	2.01	0.42
1:E:365:LEU:HD23	1:F:559:PHE:CE2	2.54	0.42
1:B:512:LYS:HB3	1:B:513:LEU:H	1.49	0.42
1:A:522:ARG:O	1:A:526:ILE:HG12	2.18	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:G:458:PRO:HA	1:G:471:LEU:O	2.19	0.42
1:G:258:ILE:HD13	1:G:264:TYR:HB2	2.01	0.42
1:B:316:ARG:HB3	1:B:335:TYR:CE1	2.54	0.42
1:C:248:ASP:OD1	1:C:250:ILE:HG12	2.19	0.42
1:H:384:LEU:HD21	1:H:494:ARG:CZ	2.49	0.42
1:F:444:MET:CE	1:F:486:LEU:HD22	2.48	0.42
1:B:391:PHE:CD2	1:B:408:ALA:HB2	2.54	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:H:287:ALA:O	1:H:290:ILE:HD13	2.19	0.42
1:A:419:LEU:HD12	1:A:419:LEU:HA	1.89	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:H:419:LEU:HD12	1:H:419:LEU:HA	1.75	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:B:265:PRO:O	1:B:268:MET:N	2.52	0.42
1:H:340:LEU:HD12	1:H:340:LEU:N	2.34	0.42
1:A:533:ARG:O	1:A:536:GLU:HB2	2.20	0.42
1:A:447:GLY:O	1:A:540:ARG:NH2	2.52	0.42
1:C:479:VAL:HG11	1:C:538:VAL:CG2	2.50	0.42
1:A:435:VAL:O	1:A:438:GLU:HG2	2.19	0.42
1:C:414:TYR:CG	1:C:419:LEU:HD13	2.55	0.42
1:D:312:CYS:HB3	1:D:415:LEU:HD13	2.01	0.42
1:C:340:LEU:HD12	1:C:340:LEU:N	2.35	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:G:546:LYS:C	1:G:548:GLU:H	2.23	0.42
1:D:404:VAL:CG2	1:D:416:PRO:HA	2.44	0.42
1:H:471:LEU:HD12	1:H:495:VAL:HA	2.02	0.42
1:H:412:LEU:O	1:H:463:ILE:HB	2.20	0.42
1:E:376:SER:OG	1:E:410:SER:HB3	2.20	0.42
1:D:248:ASP:OD1	1:D:250:ILE:HG12	2.19	0.42
1:D:528:GLU:O	1:D:532:LYS:HB2	2.20	0.42

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

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

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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:B:501:GLN:OE1	2:B:903:DTT:S4	2.79	0.40
1:A:397:ALA:HB2	1:A:486:LEU:O	2.22	0.40
1:F:290:ILE:HG22	1:F:342:LEU:CD1	2.51	0.40
1:B:282:ASP:HB3	1:B:313:VAL:HG23	2.01	0.40
1:H:444:MET:CE	1:H:486:LEU:HD22	2.50	0.40
1:E:344:PHE:HB3	1:E:364:MET:HE3	2.04	0.40
1:C:413:GLY:HA3	1:C:464:GLN:HB3	2.02	0.40
1:E:530:ILE:O	1:E:534:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/339 (88%)	265 (89%)	23 (8%)	10 (3%)	5	16
1	B	294/339 (87%)	261 (89%)	25 (8%)	8 (3%)	6	22
1	C	294/339 (87%)	264 (90%)	24 (8%)	6 (2%)	9	30
1	D	298/339 (88%)	269 (90%)	19 (6%)	10 (3%)	5	16
1	E	299/339 (88%)	267 (89%)	21 (7%)	11 (4%)	4	14
1	F	294/339 (87%)	262 (89%)	25 (8%)	7 (2%)	7	25
1	G	298/339 (88%)	266 (89%)	23 (8%)	9 (3%)	5	19
1	H	294/339 (87%)	259 (88%)	29 (10%)	6 (2%)	9	30
All	All	2369/2712 (87%)	2113 (89%)	189 (8%)	67 (3%)	6	21

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ARG

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Mol	Chain	Res	Type
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 ⓘ

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%)	7	19
1	B	269/298 (90%)	235 (87%)	34 (13%)	5	14
1	C	269/298 (90%)	231 (86%)	38 (14%)	4	11
1	D	273/298 (92%)	241 (88%)	32 (12%)	7	17
1	E	274/298 (92%)	241 (88%)	33 (12%)	6	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	269/298 (90%)	237 (88%)	32 (12%)	6	17
1	G	273/298 (92%)	245 (90%)	28 (10%)	9	24
1	H	269/298 (90%)	228 (85%)	41 (15%)	3	9
All	All	2169/2384 (91%)	1900 (88%)	269 (12%)	6	15

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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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

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

Mol	Chain	Res	Type
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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Mol	Chain	Res	Type
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 carbohydrates 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	A	900	1	7,7,7	0.77	0	4,8,8	0.87	0
2	DTT	A	901	1	7,7,7	1.06	0	4,8,8	1.18	1 (25%)
2	DTT	A	902	1	7,7,7	0.94	0	4,8,8	0.94	0
2	DTT	A	903	1	7,7,7	0.77	0	4,8,8	0.85	0
2	DTT	B	900	1	7,7,7	0.79	0	4,8,8	0.86	0
2	DTT	B	901	1	7,7,7	0.91	0	4,8,8	1.14	1 (25%)
2	DTT	B	902	1	7,7,7	0.96	0	4,8,8	0.83	0
2	DTT	B	903	1	7,7,7	1.04	1 (14%)	4,8,8	0.20	0
2	DTT	C	900	1	7,7,7	0.81	0	4,8,8	0.56	0
2	DTT	C	901	1	7,7,7	0.86	0	4,8,8	0.53	0
2	DTT	C	902	1	7,7,7	0.95	0	4,8,8	0.69	0
2	DTT	C	903	1	7,7,7	1.44	1 (14%)	4,8,8	1.25	1 (25%)
2	DTT	D	900	1	7,7,7	0.63	0	4,8,8	0.61	0
2	DTT	D	901	1	7,7,7	1.02	0	4,8,8	0.95	0
2	DTT	D	902	1	7,7,7	0.99	0	4,8,8	0.82	0
2	DTT	E	900	1	7,7,7	0.77	0	4,8,8	0.75	0
2	DTT	E	901	1	7,7,7	1.09	0	4,8,8	1.10	1 (25%)
2	DTT	F	900	1	7,7,7	0.83	0	4,8,8	0.89	0
2	DTT	F	901	1	7,7,7	0.94	0	4,8,8	1.04	0
2	DTT	F	902	1	7,7,7	0.79	0	4,8,8	0.61	0
2	DTT	F	903	1	7,7,7	1.42	1 (14%)	4,8,8	0.59	0
2	DTT	G	900	1	7,7,7	0.75	0	4,8,8	0.97	0
2	DTT	G	901	1	7,7,7	1.06	0	4,8,8	1.15	1 (25%)
2	DTT	G	902	1	7,7,7	0.98	0	4,8,8	0.50	0
2	DTT	H	900	1	7,7,7	0.82	0	4,8,8	0.81	0
2	DTT	H	901	1	7,7,7	0.99	0	4,8,8	1.36	1 (25%)
2	DTT	H	902	1	7,7,7	1.02	0	4,8,8	1.16	1 (25%)
2	DTT	H	903	1	7,7,7	1.07	0	4,8,8	0.88	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	A	900	1	-	0/8/8/8	0/0/0/0
2	DTT	A	901	1	-	0/8/8/8	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DTT	A	902	1	-	0/8/8/8	0/0/0/0
2	DTT	A	903	1	-	0/8/8/8	0/0/0/0
2	DTT	B	900	1	-	0/8/8/8	0/0/0/0
2	DTT	B	901	1	-	0/8/8/8	0/0/0/0
2	DTT	B	902	1	-	0/8/8/8	0/0/0/0
2	DTT	B	903	1	-	0/8/8/8	0/0/0/0
2	DTT	C	900	1	-	0/8/8/8	0/0/0/0
2	DTT	C	901	1	-	0/8/8/8	0/0/0/0
2	DTT	C	902	1	-	0/8/8/8	0/0/0/0
2	DTT	C	903	1	-	0/8/8/8	0/0/0/0
2	DTT	D	900	1	-	0/8/8/8	0/0/0/0
2	DTT	D	901	1	-	0/8/8/8	0/0/0/0
2	DTT	D	902	1	-	0/8/8/8	0/0/0/0
2	DTT	E	900	1	-	0/8/8/8	0/0/0/0
2	DTT	E	901	1	-	0/8/8/8	0/0/0/0
2	DTT	F	900	1	-	0/8/8/8	0/0/0/0
2	DTT	F	901	1	-	0/8/8/8	0/0/0/0
2	DTT	F	902	1	-	0/8/8/8	0/0/0/0
2	DTT	F	903	1	-	0/8/8/8	0/0/0/0
2	DTT	G	900	1	-	0/8/8/8	0/0/0/0
2	DTT	G	901	1	-	0/8/8/8	0/0/0/0
2	DTT	G	902	1	-	0/8/8/8	0/0/0/0
2	DTT	H	900	1	-	0/8/8/8	0/0/0/0
2	DTT	H	901	1	-	0/8/8/8	0/0/0/0
2	DTT	H	902	1	-	0/8/8/8	0/0/0/0
2	DTT	H	903	1	-	0/8/8/8	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	903	DTT	C4-C3	2.17	1.56	1.51
2	F	903	DTT	C4-S4	2.86	1.87	1.81
2	C	903	DTT	C1-C2	2.93	1.58	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	901	DTT	C3-C4-S4	2.03	117.28	113.91
2	H	902	DTT	C3-C4-S4	2.05	117.32	113.91
2	G	901	DTT	C3-C4-S4	2.10	117.39	113.91
2	B	901	DTT	C3-C4-S4	2.14	117.47	113.91
2	C	903	DTT	C3-C4-S4	2.28	117.70	113.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	DTT	C3-C4-S4	2.30	117.73	113.91
2	H	901	DTT	C3-C4-S4	2.66	118.32	113.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 30 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	306/339 (90%)	0.06	15 (4%) 33 27	31, 56, 125, 134	0
1	B	302/339 (89%)	-0.03	9 (2%) 54 47	32, 58, 115, 130	0
1	C	302/339 (89%)	0.13	13 (4%) 39 32	29, 60, 126, 142	0
1	D	306/339 (90%)	0.20	19 (6%) 24 17	31, 63, 130, 147	0
1	E	307/339 (90%)	0.21	21 (6%) 20 14	28, 56, 128, 146	0
1	F	302/339 (89%)	0.12	14 (4%) 36 30	32, 64, 127, 139	0
1	G	306/339 (90%)	0.09	19 (6%) 24 17	30, 58, 128, 136	0
1	H	302/339 (89%)	0.24	19 (6%) 23 17	43, 78, 121, 144	0
All	All	2433/2712 (89%)	0.13	129 (5%) 30 24	28, 62, 126, 147	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	356	TYR	8.6
1	E	574	LEU	7.9
1	E	572	LEU	7.9
1	C	353	PRO	7.7
1	D	574	LEU	6.8
1	C	356	TYR	6.7
1	D	350	GLU	6.4
1	E	350	GLU	6.4
1	C	307	ALA	6.3
1	E	571	ASP	6.2
1	E	349	GLU	6.0
1	E	573	LYS	6.0
1	B	353	PRO	5.9
1	D	573	LYS	5.8
1	G	350	GLU	5.8
1	A	571	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	H	353	PRO	5.8
1	H	355	ASN	5.7
1	F	356	TYR	5.6
1	D	349	GLU	5.5
1	B	356	TYR	5.5
1	A	572	LEU	5.4
1	G	571	ASP	5.1
1	D	571	ASP	5.1
1	F	353	PRO	4.9
1	D	514	LYS	4.8
1	E	307	ALA	4.8
1	D	572	LEU	4.8
1	C	547	GLN	4.8
1	G	518	GLU	4.7
1	C	354	ASP	4.7
1	E	518	GLU	4.6
1	H	319	ARG	4.6
1	G	387	LYS	4.5
1	G	572	LEU	4.5
1	G	544	THR	4.4
1	B	355	ASN	4.4
1	D	544	THR	4.3
1	C	513	LEU	4.3
1	A	236	LYS	4.2
1	E	544	THR	4.1
1	F	307	ALA	4.1
1	D	547	GLN	4.1
1	A	350	GLU	3.9
1	H	354	ASP	3.9
1	G	509	PRO	3.9
1	E	547	GLN	3.8
1	E	513	LEU	3.8
1	A	544	THR	3.8
1	D	550	SER	3.8
1	F	549	VAL	3.6
1	A	546	LYS	3.4
1	D	508	ALA	3.4
1	F	354	ASP	3.3
1	C	236	LYS	3.3
1	F	550	SER	3.3
1	F	236	LYS	3.3
1	G	361	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	546	LYS	3.2
1	H	389	PRO	3.2
1	H	351	ALA	3.2
1	A	518	GLU	3.1
1	C	352	ARG	3.1
1	G	574	LEU	3.0
1	F	547	GLN	3.0
1	F	553	CYS	3.0
1	D	542	SER	2.9
1	D	361	GLY	2.9
1	A	387	LYS	2.9
1	E	386	GLN	2.9
1	H	543	GLU	2.9
1	B	236	LYS	2.9
1	A	349	GLU	2.9
1	H	518	GLU	2.9
1	A	509	PRO	2.9
1	E	542	SER	2.8
1	E	508	ALA	2.8
1	E	309	SER	2.8
1	G	309	SER	2.8
1	E	546	LYS	2.8
1	E	348	PRO	2.8
1	A	542	SER	2.7
1	D	307	ALA	2.7
1	G	349	GLU	2.7
1	H	549	VAL	2.7
1	G	573	LYS	2.7
1	D	570	ALA	2.7
1	D	549	VAL	2.6
1	C	355	ASN	2.6
1	E	387	LYS	2.6
1	G	542	SER	2.6
1	H	544	THR	2.6
1	G	513	LEU	2.5
1	C	549	VAL	2.5
1	E	361	GLY	2.5
1	D	236	LYS	2.5
1	G	508	ALA	2.5
1	F	319	ARG	2.4
1	A	543	GLU	2.4
1	B	543	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	574	LEU	2.4
1	F	352	ARG	2.4
1	B	348	PRO	2.4
1	G	546	LYS	2.4
1	H	387	LYS	2.4
1	B	319	ARG	2.4
1	H	384	LEU	2.3
1	B	350	GLU	2.3
1	G	548	GLU	2.3
1	F	355	ASN	2.3
1	C	545	VAL	2.3
1	C	319	ARG	2.3
1	D	295	PRO	2.3
1	F	513	LEU	2.3
1	H	307	ALA	2.2
1	A	573	LYS	2.2
1	B	513	LEU	2.2
1	H	388	SER	2.2
1	H	513	LEU	2.1
1	A	510	THR	2.1
1	C	548	GLU	2.1
1	G	545	VAL	2.1
1	H	565	ASP	2.1
1	E	543	GLU	2.1
1	H	545	VAL	2.1
1	H	333	VAL	2.1
1	D	377	TYR	2.0
1	E	550	SER	2.0
1	G	385	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	DTT	D	902	8/8	0.62	0.66	19.08	135,141,142,143	0
2	DTT	A	902	8/8	0.40	0.68	6.94	136,140,143,146	0
2	DTT	C	903	8/8	0.78	0.52	6.60	125,137,140,143	0
2	DTT	C	901	8/8	0.80	0.31	5.66	96,104,110,114	0
2	DTT	G	902	8/8	0.74	0.60	5.39	130,131,132,132	0
2	DTT	G	900	8/8	0.85	0.26	5.35	71,74,85,91	0
2	DTT	B	903	8/8	0.80	0.52	4.66	125,135,139,141	0
2	DTT	B	901	8/8	0.80	0.24	4.56	85,90,97,100	0
2	DTT	B	902	8/8	0.86	0.35	3.32	98,106,112,117	0
2	DTT	F	901	8/8	0.79	0.26	3.26	94,98,103,105	0
2	DTT	H	901	8/8	0.65	0.28	2.72	112,117,120,121	0
2	DTT	B	900	8/8	0.77	0.25	2.68	80,83,89,97	0
2	DTT	H	900	8/8	0.65	0.26	1.78	104,105,109,112	0
2	DTT	H	902	8/8	0.78	0.28	1.63	96,100,104,110	0
2	DTT	A	900	8/8	0.90	0.21	1.47	74,77,84,89	0
2	DTT	F	900	8/8	0.86	0.23	1.47	82,89,95,102	0
2	DTT	F	902	8/8	0.77	0.34	1.45	119,120,121,124	0
2	DTT	D	900	8/8	0.83	0.23	1.41	71,75,81,88	0
2	DTT	E	900	8/8	0.82	0.21	1.40	74,77,82,87	0
2	DTT	F	903	8/8	0.76	0.27	1.23	129,136,138,140	0
2	DTT	C	902	8/8	0.86	0.23	0.34	102,107,110,115	0
2	DTT	C	900	8/8	0.85	0.17	-0.02	77,83,90,99	0
2	DTT	H	903	8/8	0.75	0.19	-0.69	135,139,141,142	0
2	DTT	A	901	8/8	0.74	0.39	-	99,107,111,111	0
2	DTT	D	901	8/8	0.64	0.52	-	108,115,119,120	0
2	DTT	E	901	8/8	0.73	0.26	-	104,112,115,116	0
2	DTT	G	901	8/8	0.71	0.41	-	103,106,109,110	0
2	DTT	A	903	8/8	0.72	0.41	-	124,136,139,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.