



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:50 AM GMT

PDB ID : 2OCP  
Title : Crystal Structure of Human Deoxyguanosine Kinase  
Authors : Johansson, K.; Ramaswamy, S.; Ljungkrantz, C.; Knecht, W.; Piskur, J.;  
Munch-Petersen, B.; Eriksson, S.; Eklund, H.  
Deposited on : 2006-12-21  
Resolution : 2.80 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 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

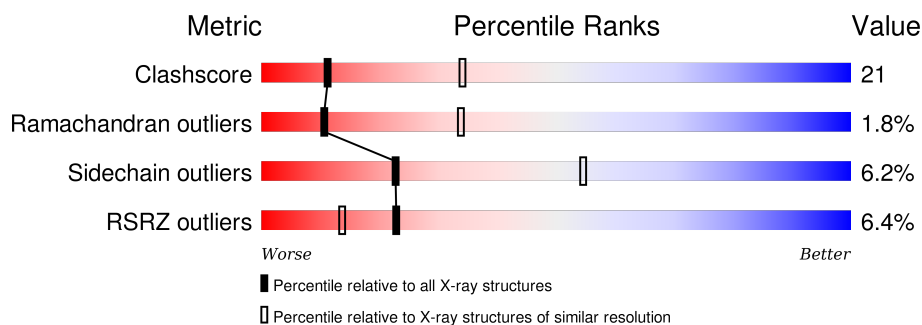
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	241	<div> <div>9%</div> <div> <div>57%</div> <div>35%</div> <div>• 5%</div> </div> </div>
1	B	241	<div> <div>4%</div> <div> <div>55%</div> <div>36%</div> <div>• 5%</div> </div> </div>
1	C	241	<div> <div>6%</div> <div> <div>57%</div> <div>34%</div> <div>• 5%</div> </div> </div>
1	D	241	<div> <div>3%</div> <div> <div>58%</div> <div>34%</div> <div>• 5%</div> </div> </div>
1	E	241	<div> <div>7%</div> <div> <div>55%</div> <div>37%</div> <div>• 5%</div> </div> </div>
1	F	241	<div> <div>7%</div> <div> <div>56%</div> <div>36%</div> <div>• 5%</div> </div> </div>
1	G	241	<div> <div>6%</div> <div> <div>55%</div> <div>37%</div> <div>• 5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	H	241	<div><div></div><div>7%</div><div>56%</div><div>36%</div><div>• 5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15832 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.

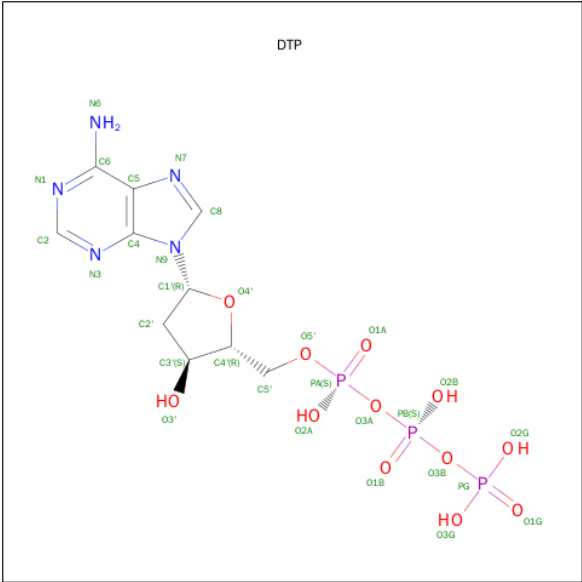
- Molecule 1 is a protein called Deoxyguanosine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	B	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	C	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	D	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	E	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	F	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	G	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			
1	H	229	Total	C	N	O	S	0	0	0
			1924	1249	326	344	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ASN	THR	variant	UNP Q16854
B	83	ASN	THR	variant	UNP Q16854
C	83	ASN	THR	variant	UNP Q16854
D	83	ASN	THR	variant	UNP Q16854
E	83	ASN	THR	variant	UNP Q16854
F	83	ASN	THR	variant	UNP Q16854
G	83	ASN	THR	variant	UNP Q16854
H	83	ASN	THR	variant	UNP Q16854

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula:  $C_{10}H_{16}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	C	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	E	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	F	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	G	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	H	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	B	25	Total	O	0	0
			25	25		
3	C	25	Total	O	0	0
			25	25		
3	D	25	Total	O	0	0
			25	25		

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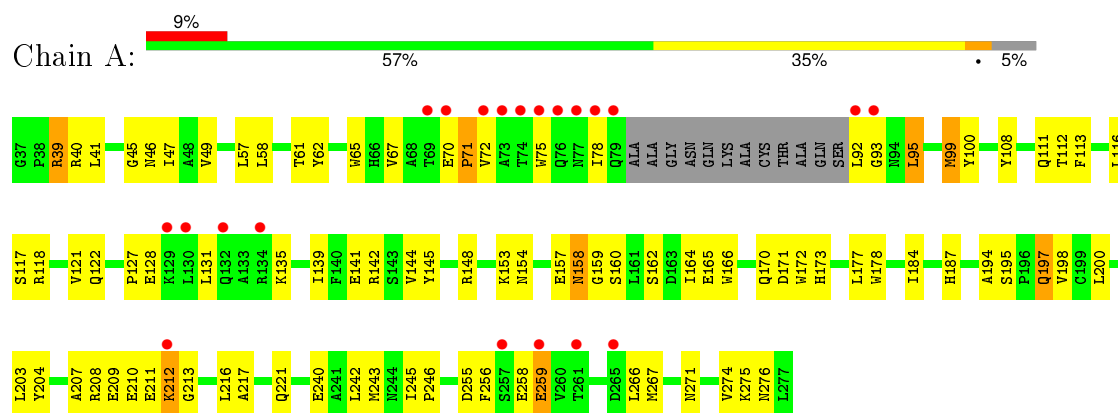
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	25	Total 25	O 25	0	0
3	F	25	Total 25	O 25	0	0
3	G	25	Total 25	O 25	0	0
3	H	25	Total 25	O 25	0	0

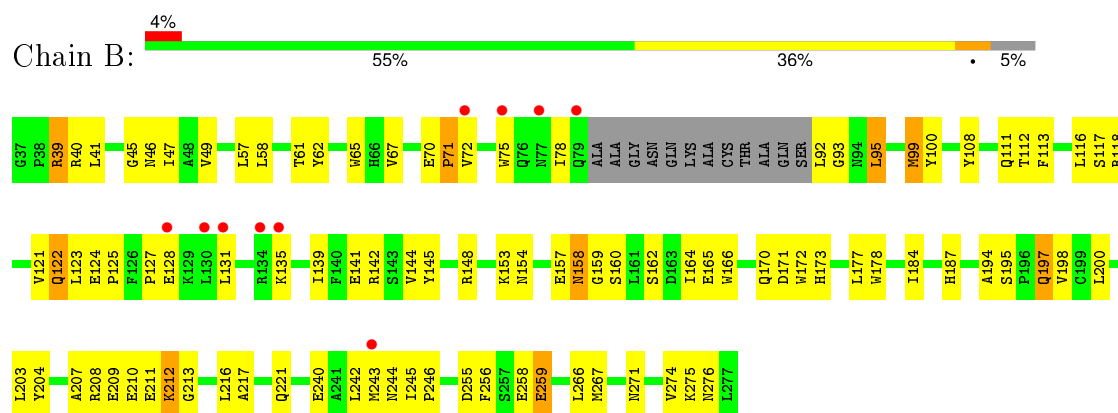
### 3 Residue-property plots

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.

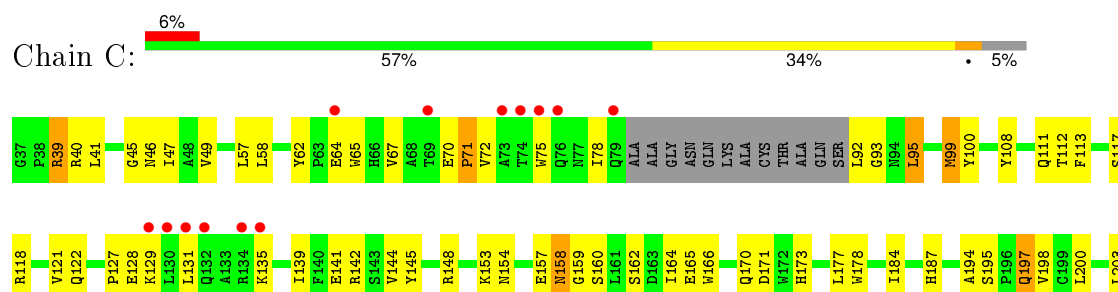
#### • Molecule 1: Deoxyguanosine kinase

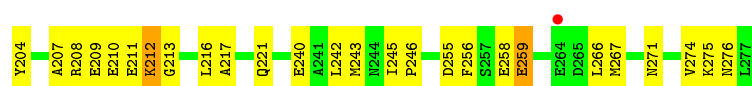


#### • Molecule 1: Deoxyguanosine kinase

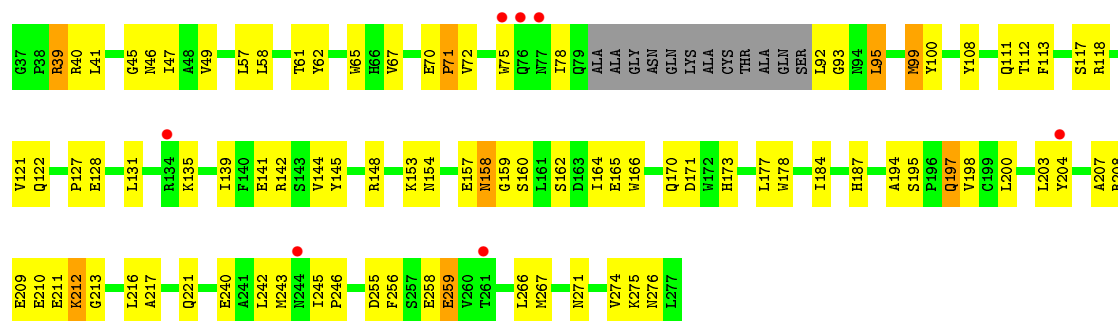


#### • Molecule 1: Deoxyguanosine kinase

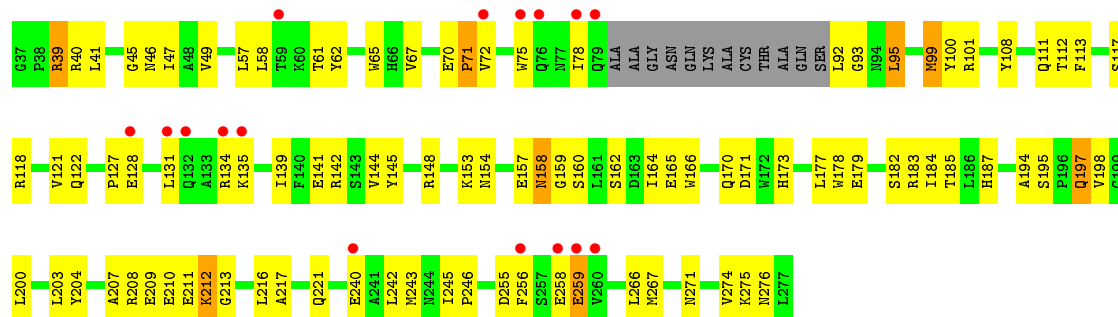




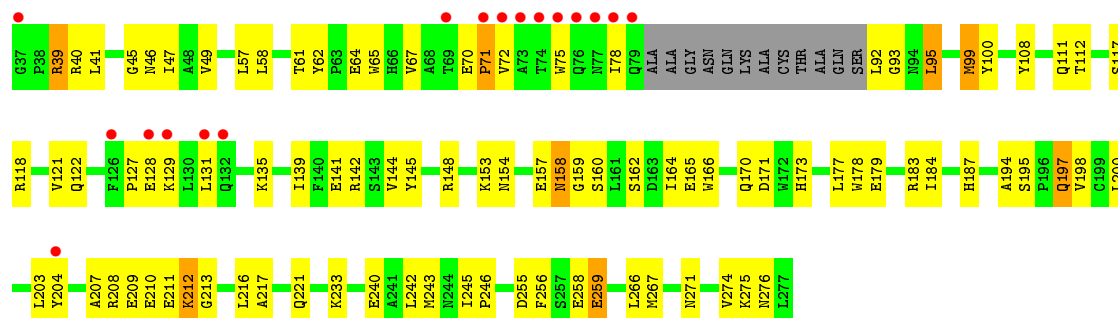
• Molecule 1: Deoxyguanosine kinase



• Molecule 1: Deoxyguanosine kinase



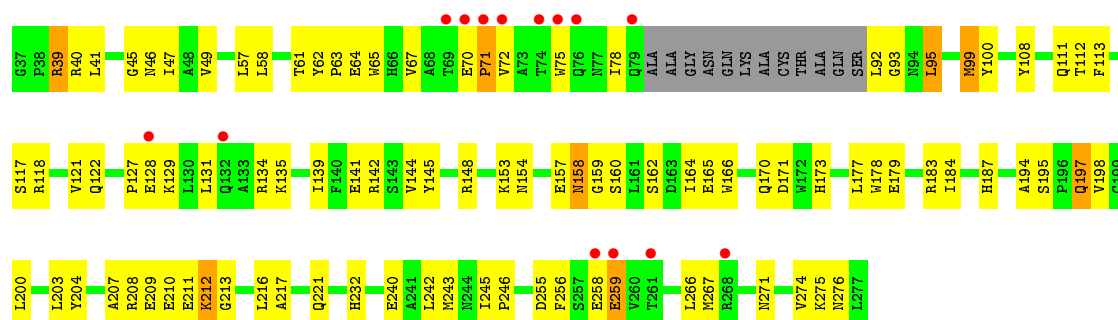
• Molecule 1: Deoxyguanosine kinase



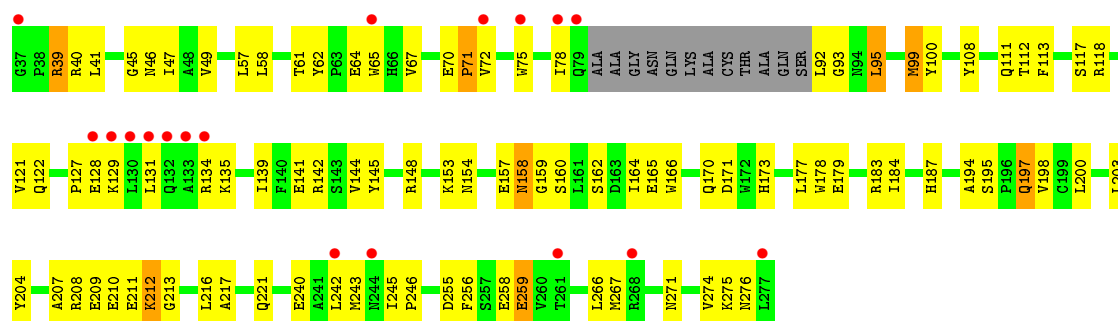
• Molecule 1: Deoxyguanosine kinase







• Molecule 1: Deoxyguanosine kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.18Å 120.03Å 154.35Å 90.00° 90.68° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 38.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (30.00-2.80) 97.5 (38.77-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.265 , 0.277 0.285 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	35.1	Xtriage
Anisotropy	0.976	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 43.4	EDS
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	2 of 59766 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	15832	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DTP

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	0.40	0/1976	0.61	0/2676
1	B	0.40	0/1976	0.61	0/2676
1	C	0.40	0/1976	0.61	0/2676
1	D	0.40	0/1976	0.61	0/2676
1	E	0.40	0/1976	0.61	0/2676
1	F	0.40	0/1976	0.61	0/2676
1	G	0.40	0/1976	0.61	0/2676
1	H	0.40	0/1976	0.61	0/2676
All	All	0.40	0/15808	0.61	0/21408

There are no bond length outliers.

There are no bond angle outliers.

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	1924	0	1899	81	1
1	B	1924	0	1899	90	3
1	C	1924	0	1899	76	10
1	D	1924	0	1899	77	2
1	E	1924	0	1899	87	11

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1924	0	1899	83	3
1	G	1924	0	1899	83	7
1	H	1924	0	1899	82	3
2	A	30	0	12	1	0
2	B	30	0	12	3	0
2	C	30	0	12	2	0
2	D	30	0	12	2	0
2	E	30	0	12	1	0
2	F	30	0	12	2	0
2	G	30	0	12	3	0
2	H	30	0	12	3	0
3	A	25	0	0	5	0
3	B	25	0	0	5	0
3	C	25	0	0	5	0
3	D	25	0	0	5	0
3	E	25	0	0	5	0
3	F	25	0	0	5	0
3	G	25	0	0	5	0
3	H	25	0	0	5	0
All	All	15832	0	15288	639	20

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 (639) 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:B:244:ASN:CB	1:E:134:ARG:HH22	1.36	1.34
1:B:244:ASN:HB3	1:E:134:ARG:NH2	1.58	1.16
1:B:244:ASN:CB	1:E:134:ARG:NH2	2.13	1.08
1:H:40:ARG:H	1:H:187:HIS:HD2	1.01	1.00
1:G:40:ARG:H	1:G:187:HIS:HD2	1.01	1.00
1:B:244:ASN:HB3	1:E:134:ARG:HH22	0.84	0.99
1:E:40:ARG:H	1:E:187:HIS:HD2	1.01	0.99
1:B:40:ARG:H	1:B:187:HIS:HD2	1.01	0.98
1:C:40:ARG:H	1:C:187:HIS:HD2	1.01	0.95
1:A:40:ARG:H	1:A:187:HIS:HD2	1.01	0.93
1:F:40:ARG:H	1:F:187:HIS:HD2	1.01	0.93
1:D:40:ARG:H	1:D:187:HIS:HD2	1.01	0.92
1:C:40:ARG:H	1:C:187:HIS:CD2	1.88	0.92
1:A:40:ARG:H	1:A:187:HIS:CD2	1.88	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:ARG:H	1:E:187:HIS:CD2	1.88	0.91
1:D:40:ARG:H	1:D:187:HIS:CD2	1.88	0.91
1:B:40:ARG:H	1:B:187:HIS:CD2	1.88	0.91
1:F:40:ARG:H	1:F:187:HIS:CD2	1.88	0.91
1:G:40:ARG:H	1:G:187:HIS:CD2	1.88	0.90
1:B:244:ASN:CG	1:E:134:ARG:HH22	1.75	0.90
1:H:40:ARG:H	1:H:187:HIS:CD2	1.88	0.90
1:B:244:ASN:CG	1:E:134:ARG:NH2	2.28	0.86
1:C:58:LEU:HD23	1:C:267:MET:HE1	1.57	0.85
1:F:118:ARG:HH12	2:F:301:DTP:HN61	1.25	0.84
1:A:118:ARG:HH12	2:A:301:DTP:HN61	1.26	0.83
1:G:118:ARG:HH12	2:G:301:DTP:HN61	1.27	0.83
1:B:118:ARG:HH12	2:B:301:DTP:HN61	1.27	0.82
1:H:58:LEU:HD23	1:H:267:MET:HE1	1.62	0.81
1:D:118:ARG:HH12	2:D:301:DTP:HN61	1.23	0.81
1:F:58:LEU:HD23	1:F:267:MET:HE1	1.62	0.81
1:E:118:ARG:HH12	2:E:301:DTP:HN61	1.28	0.80
1:C:118:ARG:HH12	2:C:301:DTP:HN61	1.26	0.80
1:B:40:ARG:N	1:B:187:HIS:HD2	1.80	0.80
1:A:158:ASN:HD22	1:A:158:ASN:C	1.86	0.79
1:F:158:ASN:HD22	1:F:158:ASN:C	1.86	0.79
1:D:158:ASN:C	1:D:158:ASN:HD22	1.86	0.79
1:H:128:GLU:HA	1:H:131:LEU:HD12	1.64	0.79
1:C:40:ARG:N	1:C:187:HIS:HD2	1.79	0.79
1:C:158:ASN:C	1:C:158:ASN:HD22	1.86	0.79
1:D:128:GLU:HA	1:D:131:LEU:HD12	1.64	0.79
1:H:118:ARG:HH12	2:H:301:DTP:HN61	1.31	0.78
1:B:128:GLU:HA	1:B:131:LEU:HD12	1.64	0.78
1:G:40:ARG:N	1:G:187:HIS:HD2	1.80	0.78
1:C:127:PRO:O	1:C:131:LEU:HG	1.84	0.78
1:C:58:LEU:HA	1:C:267:MET:HE1	1.65	0.78
1:B:158:ASN:C	1:B:158:ASN:HD22	1.86	0.78
1:A:40:ARG:N	1:A:187:HIS:HD2	1.80	0.77
1:H:127:PRO:O	1:H:131:LEU:HG	1.84	0.77
1:B:58:LEU:HD23	1:B:267:MET:HE1	1.67	0.77
1:C:128:GLU:HA	1:C:131:LEU:HD12	1.64	0.77
1:F:127:PRO:O	1:F:131:LEU:HG	1.84	0.77
1:H:40:ARG:N	1:H:187:HIS:HD2	1.80	0.77
1:E:40:ARG:N	1:E:187:HIS:HD2	1.80	0.77
1:E:128:GLU:HA	1:E:131:LEU:HD12	1.65	0.77
1:H:158:ASN:HD22	1:H:158:ASN:C	1.86	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:O	1:A:131:LEU:HG	1.84	0.77
1:D:127:PRO:O	1:D:131:LEU:HG	1.84	0.77
1:D:40:ARG:N	1:D:187:HIS:HD2	1.80	0.76
1:F:128:GLU:HA	1:F:131:LEU:HD12	1.64	0.76
1:A:128:GLU:HA	1:A:131:LEU:HD12	1.64	0.76
1:E:158:ASN:HD22	1:E:158:ASN:C	1.86	0.76
1:G:128:GLU:HA	1:G:131:LEU:HD12	1.64	0.76
1:G:158:ASN:C	1:G:158:ASN:HD22	1.86	0.76
1:B:127:PRO:O	1:B:131:LEU:HG	1.84	0.76
1:F:40:ARG:N	1:F:187:HIS:HD2	1.79	0.76
1:G:127:PRO:O	1:G:131:LEU:HG	1.84	0.76
1:E:58:LEU:HD23	1:E:267:MET:HE1	1.67	0.76
1:C:78:ILE:HG13	1:D:164:ILE:HD12	1.67	0.75
1:E:127:PRO:O	1:E:131:LEU:HG	1.84	0.75
1:B:78:ILE:HD11	1:B:95:LEU:HB2	1.70	0.73
1:A:78:ILE:HD11	1:A:95:LEU:HB2	1.71	0.73
1:A:58:LEU:HD23	1:A:267:MET:HE3	1.70	0.73
1:D:78:ILE:HD11	1:D:95:LEU:HB2	1.71	0.73
1:C:78:ILE:HD11	1:C:95:LEU:HB2	1.70	0.73
1:E:78:ILE:HD11	1:E:95:LEU:HB2	1.71	0.73
1:F:78:ILE:HD11	1:F:95:LEU:HB2	1.71	0.72
1:H:78:ILE:HD11	1:H:95:LEU:HB2	1.70	0.72
1:G:78:ILE:HD11	1:G:95:LEU:HB2	1.70	0.71
1:B:40:ARG:HH11	1:B:40:ARG:HG3	1.55	0.71
1:F:40:ARG:HG3	1:F:40:ARG:HH11	1.56	0.71
1:G:128:GLU:HA	1:G:131:LEU:CD1	2.21	0.70
1:D:58:LEU:HD23	1:D:267:MET:HE3	1.73	0.70
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.55	0.70
1:E:128:GLU:HA	1:E:131:LEU:CD1	2.21	0.70
1:H:178:TRP:HB2	3:H:808:HOH:O	1.92	0.70
1:E:40:ARG:HH11	1:E:40:ARG:HG3	1.56	0.70
1:D:40:ARG:HH11	1:D:40:ARG:HG3	1.55	0.70
1:A:40:ARG:HG3	1:A:40:ARG:HH11	1.55	0.70
1:A:128:GLU:HA	1:A:131:LEU:CD1	2.21	0.70
1:H:40:ARG:HG3	1:H:40:ARG:HH11	1.55	0.70
1:H:128:GLU:HA	1:H:131:LEU:CD1	2.21	0.70
1:F:128:GLU:HA	1:F:131:LEU:CD1	2.21	0.70
1:D:128:GLU:HA	1:D:131:LEU:CD1	2.21	0.69
1:C:128:GLU:HA	1:C:131:LEU:CD1	2.21	0.69
1:D:58:LEU:HA	1:D:267:MET:HE1	1.74	0.69
1:G:178:TRP:HB2	3:G:708:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:LEU:HA	1:G:267:MET:HE1	1.74	0.69
1:B:128:GLU:HA	1:B:131:LEU:CD1	2.21	0.69
1:G:58:LEU:HD23	1:G:267:MET:HE3	1.74	0.69
1:F:178:TRP:HB2	3:F:608:HOH:O	1.92	0.69
1:G:40:ARG:HH11	1:G:40:ARG:HG3	1.56	0.69
1:A:178:TRP:HB2	3:A:307:HOH:O	1.92	0.69
1:B:178:TRP:HB2	3:B:309:HOH:O	1.92	0.68
1:D:178:TRP:HB2	3:D:309:HOH:O	1.92	0.68
1:E:178:TRP:HB2	3:E:508:HOH:O	1.92	0.68
1:C:178:TRP:HB2	3:C:308:HOH:O	1.92	0.67
1:H:57:LEU:HD22	1:H:267:MET:SD	2.35	0.67
1:E:57:LEU:HD22	1:E:267:MET:SD	2.35	0.67
1:B:57:LEU:HD22	1:B:267:MET:SD	2.35	0.67
1:F:57:LEU:HD22	1:F:267:MET:SD	2.35	0.67
1:A:70:GLU:HB2	1:A:141:GLU:HB2	1.77	0.67
1:G:57:LEU:HD22	1:G:267:MET:SD	2.35	0.67
1:E:99:MET:HG3	1:E:100:TYR:N	2.10	0.66
1:A:58:LEU:HA	1:A:267:MET:HE1	1.76	0.66
1:G:99:MET:HG3	1:G:100:TYR:N	2.10	0.66
1:C:70:GLU:HB2	1:C:141:GLU:HB2	1.77	0.66
1:A:57:LEU:HD22	1:A:267:MET:SD	2.35	0.66
1:D:57:LEU:HD22	1:D:267:MET:SD	2.35	0.66
1:D:70:GLU:HB2	1:D:141:GLU:HB2	1.77	0.66
1:F:70:GLU:HB2	1:F:141:GLU:HB2	1.77	0.66
1:G:70:GLU:HB2	1:G:141:GLU:HB2	1.77	0.66
1:C:57:LEU:HD22	1:C:267:MET:SD	2.35	0.66
1:E:70:GLU:HB2	1:E:141:GLU:HB2	1.77	0.66
1:B:99:MET:HG3	1:B:100:TYR:N	2.10	0.66
1:F:99:MET:HG3	1:F:100:TYR:N	2.10	0.66
1:H:99:MET:HG3	1:H:100:TYR:N	2.10	0.65
1:D:99:MET:HG3	1:D:100:TYR:N	2.10	0.65
1:H:70:GLU:HB2	1:H:141:GLU:HB2	1.77	0.65
1:E:58:LEU:HA	1:E:267:MET:HE2	1.79	0.65
1:A:99:MET:HG3	1:A:100:TYR:N	2.10	0.65
1:C:99:MET:HG3	1:C:100:TYR:N	2.10	0.64
1:B:70:GLU:HB2	1:B:141:GLU:HB2	1.77	0.64
1:B:58:LEU:HA	1:B:267:MET:HE2	1.79	0.63
1:D:158:ASN:ND2	1:D:158:ASN:C	2.53	0.62
1:E:158:ASN:ND2	1:E:158:ASN:C	2.53	0.62
1:F:158:ASN:ND2	1:F:158:ASN:C	2.53	0.62
1:B:158:ASN:C	1:B:158:ASN:ND2	2.53	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:158:ASN:ND2	1:H:158:ASN:C	2.53	0.61
1:G:158:ASN:C	1:G:158:ASN:ND2	2.53	0.61
1:C:158:ASN:ND2	1:C:158:ASN:C	2.53	0.61
1:H:62:TYR:OH	1:H:271:ASN:HB2	2.01	0.61
1:C:62:TYR:OH	1:C:271:ASN:HB2	2.01	0.61
1:A:158:ASN:ND2	1:A:158:ASN:C	2.53	0.61
1:A:62:TYR:OH	1:A:271:ASN:HB2	2.01	0.61
1:F:58:LEU:HA	1:F:267:MET:HE2	1.83	0.60
1:D:164:ILE:HG12	3:D:308:HOH:O	2.01	0.60
1:E:62:TYR:OH	1:E:271:ASN:HB2	2.01	0.60
1:H:164:ILE:HG12	3:H:807:HOH:O	2.01	0.60
1:G:62:TYR:OH	1:G:271:ASN:HB2	2.01	0.60
1:E:164:ILE:HG12	3:E:507:HOH:O	2.01	0.60
1:B:62:TYR:OH	1:B:271:ASN:HB2	2.01	0.60
1:G:164:ILE:HG12	3:G:707:HOH:O	2.01	0.60
1:F:62:TYR:OH	1:F:271:ASN:HB2	2.01	0.60
1:H:58:LEU:HA	1:H:267:MET:HE2	1.83	0.60
1:A:65:TRP:CH2	1:A:274:VAL:HG21	2.37	0.59
1:F:65:TRP:CH2	1:F:274:VAL:HG21	2.37	0.59
1:D:62:TYR:OH	1:D:271:ASN:HB2	2.01	0.59
1:D:65:TRP:CH2	1:D:274:VAL:HG21	2.37	0.59
1:A:164:ILE:HG12	3:A:306:HOH:O	2.01	0.59
1:B:164:ILE:HG12	3:B:308:HOH:O	2.01	0.59
1:C:195:SER:OG	1:C:198:VAL:HG23	2.03	0.59
1:C:65:TRP:CH2	1:C:274:VAL:HG21	2.37	0.59
1:E:65:TRP:CH2	1:E:274:VAL:HG21	2.37	0.59
1:F:164:ILE:HG12	3:F:607:HOH:O	2.01	0.59
1:G:70:GLU:OE1	1:G:71:PRO:HD2	2.03	0.59
1:C:164:ILE:HG12	3:C:307:HOH:O	2.01	0.59
1:G:65:TRP:CH2	1:G:274:VAL:HG21	2.37	0.59
1:H:65:TRP:CH2	1:H:274:VAL:HG21	2.37	0.58
1:E:195:SER:OG	1:E:198:VAL:HG23	2.03	0.58
1:B:78:ILE:HG12	1:B:93:GLY:O	2.03	0.58
1:A:70:GLU:OE1	1:A:71:PRO:HD2	2.03	0.58
1:F:70:GLU:OE1	1:F:71:PRO:HD2	2.03	0.58
1:F:78:ILE:HG12	1:F:93:GLY:O	2.03	0.58
1:H:70:GLU:OE1	1:H:71:PRO:HD2	2.03	0.58
1:B:65:TRP:CH2	1:B:274:VAL:HG21	2.37	0.58
1:F:195:SER:OG	1:F:198:VAL:HG23	2.03	0.58
1:C:78:ILE:HG12	1:C:93:GLY:O	2.03	0.58
1:C:70:GLU:OE1	1:C:71:PRO:HD2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:HG12	1:A:93:GLY:O	2.03	0.58
1:B:195:SER:OG	1:B:198:VAL:HG23	2.03	0.58
1:E:70:GLU:OE1	1:E:71:PRO:HD2	2.03	0.58
1:D:78:ILE:HG12	1:D:93:GLY:O	2.03	0.58
1:H:78:ILE:HG12	1:H:93:GLY:O	2.03	0.58
1:D:195:SER:OG	1:D:198:VAL:HG23	2.03	0.58
1:D:40:ARG:NH1	1:D:40:ARG:HG3	2.19	0.58
1:B:70:GLU:OE1	1:B:71:PRO:HD2	2.03	0.58
1:G:40:ARG:HG3	1:G:40:ARG:NH1	2.19	0.57
1:E:40:ARG:NH1	1:E:40:ARG:HG3	2.19	0.57
1:G:78:ILE:HG12	1:G:93:GLY:O	2.03	0.57
1:A:195:SER:OG	1:A:198:VAL:HG23	2.03	0.57
1:A:40:ARG:NH1	1:A:40:ARG:HG3	2.19	0.57
1:D:70:GLU:OE1	1:D:71:PRO:HD2	2.03	0.57
1:H:195:SER:OG	1:H:198:VAL:HG23	2.03	0.57
1:C:40:ARG:HG3	1:C:40:ARG:NH1	2.19	0.57
1:G:78:ILE:HG13	1:H:164:ILE:HD12	1.86	0.57
1:G:195:SER:OG	1:G:198:VAL:HG23	2.03	0.57
1:E:78:ILE:HG12	1:E:93:GLY:O	2.03	0.57
1:E:166:TRP:O	1:E:170:GLN:HG3	2.05	0.57
1:H:40:ARG:HG3	1:H:40:ARG:NH1	2.19	0.56
1:B:166:TRP:O	1:B:170:GLN:HG3	2.05	0.56
1:C:166:TRP:O	1:C:170:GLN:HG3	2.05	0.56
1:G:166:TRP:O	1:G:170:GLN:HG3	2.05	0.56
1:D:145:TYR:CD2	1:D:242:LEU:HD22	2.41	0.56
1:G:145:TYR:CD2	1:G:242:LEU:HD22	2.41	0.56
1:B:61:THR:HB	1:B:267:MET:HE3	1.88	0.56
1:A:166:TRP:O	1:A:170:GLN:HG3	2.05	0.56
1:H:166:TRP:O	1:H:170:GLN:HG3	2.05	0.56
1:A:145:TYR:CD2	1:A:242:LEU:HD22	2.41	0.56
1:H:61:THR:HB	1:H:267:MET:HE3	1.88	0.56
1:A:62:TYR:O	1:A:65:TRP:HB2	2.06	0.56
1:G:62:TYR:O	1:G:65:TRP:HB2	2.06	0.56
1:D:62:TYR:O	1:D:65:TRP:HB2	2.06	0.55
1:B:145:TYR:CD2	1:B:242:LEU:HD22	2.41	0.55
1:F:145:TYR:CD2	1:F:242:LEU:HD22	2.41	0.55
1:B:153:LYS:O	1:B:157:GLU:HG3	2.07	0.55
1:D:166:TRP:O	1:D:170:GLN:HG3	2.05	0.55
1:F:166:TRP:O	1:F:170:GLN:HG3	2.05	0.55
1:E:62:TYR:O	1:E:65:TRP:HB2	2.07	0.55
1:B:62:TYR:O	1:B:65:TRP:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:LYS:O	1:E:157:GLU:HG3	2.07	0.55
1:E:61:THR:HB	1:E:267:MET:HE3	1.88	0.55
1:H:153:LYS:O	1:H:157:GLU:HG3	2.07	0.55
1:C:145:TYR:CD2	1:C:242:LEU:HD22	2.41	0.55
1:C:153:LYS:O	1:C:157:GLU:HG3	2.07	0.55
1:E:145:TYR:CD2	1:E:242:LEU:HD22	2.41	0.55
1:H:145:TYR:CD2	1:H:242:LEU:HD22	2.41	0.55
1:G:212:LYS:HG3	1:G:212:LYS:O	2.07	0.55
1:B:40:ARG:HG3	1:B:40:ARG:NH1	2.19	0.55
1:D:153:LYS:O	1:D:157:GLU:HG3	2.07	0.55
1:G:58:LEU:HA	1:G:267:MET:CE	2.37	0.55
1:B:58:LEU:HA	1:B:267:MET:CE	2.37	0.54
1:H:62:TYR:O	1:H:65:TRP:HB2	2.06	0.54
1:C:62:TYR:O	1:C:65:TRP:HB2	2.06	0.54
1:A:212:LYS:O	1:A:212:LYS:HG3	2.07	0.54
1:H:212:LYS:HG3	1:H:212:LYS:O	2.07	0.54
1:F:153:LYS:O	1:F:157:GLU:HG3	2.07	0.54
1:F:61:THR:HB	1:F:267:MET:HE3	1.88	0.54
1:F:40:ARG:NH1	1:F:40:ARG:HG3	2.19	0.54
1:B:61:THR:CB	1:B:267:MET:HE3	2.38	0.54
1:H:58:LEU:HA	1:H:267:MET:CE	2.37	0.54
1:E:58:LEU:HA	1:E:267:MET:CE	2.37	0.54
1:E:203:LEU:HD23	1:E:203:LEU:O	2.08	0.54
1:H:61:THR:CB	1:H:267:MET:HE3	2.38	0.54
1:C:212:LYS:HG3	1:C:212:LYS:O	2.07	0.54
1:B:212:LYS:HG3	1:B:212:LYS:O	2.07	0.54
1:E:212:LYS:O	1:E:212:LYS:HG3	2.07	0.54
1:F:212:LYS:HG3	1:F:212:LYS:O	2.07	0.54
1:A:61:THR:CB	1:A:267:MET:HE2	2.38	0.54
1:B:71:PRO:HG2	1:B:117:SER:OG	2.08	0.54
1:G:183:ARG:NH2	1:H:179:GLU:OE1	2.33	0.54
1:F:203:LEU:HD23	1:F:203:LEU:O	2.08	0.54
1:F:58:LEU:HA	1:F:267:MET:CE	2.37	0.54
1:F:62:TYR:O	1:F:65:TRP:HB2	2.06	0.54
1:D:212:LYS:HG3	1:D:212:LYS:O	2.07	0.54
1:A:58:LEU:HA	1:A:267:MET:CE	2.37	0.53
1:G:61:THR:CB	1:G:267:MET:HE2	2.38	0.53
1:G:67:VAL:HG22	1:G:139:ILE:HB	1.90	0.53
1:A:153:LYS:O	1:A:157:GLU:HG3	2.07	0.53
1:E:61:THR:CB	1:E:267:MET:HE3	2.38	0.53
1:C:67:VAL:HG22	1:C:139:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:203:LEU:O	1:G:203:LEU:HD23	2.08	0.53
1:G:153:LYS:O	1:G:157:GLU:HG3	2.07	0.53
1:G:154:ASN:HD21	1:G:221:GLN:HE21	1.56	0.53
1:A:61:THR:HB	1:A:267:MET:HE2	1.89	0.53
1:D:61:THR:CB	1:D:267:MET:HE2	2.38	0.53
1:E:71:PRO:HG2	1:E:117:SER:OG	2.08	0.53
1:C:148:ARG:HD2	1:C:173:HIS:ND1	2.24	0.53
1:F:154:ASN:HD21	1:F:221:GLN:HE21	1.56	0.53
1:D:58:LEU:HA	1:D:267:MET:CE	2.37	0.53
1:D:61:THR:HB	1:D:267:MET:HE2	1.90	0.53
1:E:67:VAL:HG22	1:E:139:ILE:HB	1.90	0.53
1:A:154:ASN:HD21	1:A:221:GLN:HE21	1.56	0.53
1:D:148:ARG:HD2	1:D:173:HIS:ND1	2.24	0.53
1:A:71:PRO:HG2	1:A:117:SER:OG	2.08	0.53
1:D:71:PRO:HG2	1:D:117:SER:OG	2.08	0.53
1:F:67:VAL:HG22	1:F:139:ILE:HB	1.90	0.53
1:H:203:LEU:HD23	1:H:203:LEU:O	2.08	0.53
1:A:203:LEU:HD23	1:A:203:LEU:O	2.08	0.53
1:G:148:ARG:HD2	1:G:173:HIS:ND1	2.24	0.53
1:B:203:LEU:O	1:B:203:LEU:HD23	2.08	0.53
1:A:148:ARG:HD2	1:A:173:HIS:ND1	2.24	0.53
1:D:203:LEU:O	1:D:203:LEU:HD23	2.08	0.53
1:F:61:THR:CB	1:F:267:MET:HE3	2.38	0.53
1:H:71:PRO:HG2	1:H:117:SER:OG	2.08	0.53
1:B:148:ARG:HD2	1:B:173:HIS:ND1	2.24	0.53
1:E:148:ARG:HD2	1:E:173:HIS:ND1	2.24	0.53
1:H:67:VAL:HG22	1:H:139:ILE:HB	1.90	0.53
1:F:148:ARG:HD2	1:F:173:HIS:ND1	2.24	0.53
1:G:71:PRO:HG2	1:G:117:SER:OG	2.08	0.53
1:D:67:VAL:HG22	1:D:139:ILE:HB	1.90	0.52
1:C:154:ASN:HD21	1:C:221:GLN:HE21	1.56	0.52
1:F:39:ARG:HA	1:F:187:HIS:CD2	2.45	0.52
1:F:71:PRO:HG2	1:F:117:SER:OG	2.08	0.52
1:H:148:ARG:HD2	1:H:173:HIS:ND1	2.24	0.52
1:C:203:LEU:HD23	1:C:203:LEU:O	2.08	0.52
1:B:67:VAL:HG22	1:B:139:ILE:HB	1.90	0.52
1:H:39:ARG:HA	1:H:187:HIS:CD2	2.45	0.52
1:B:39:ARG:HA	1:B:187:HIS:CD2	2.45	0.52
1:E:154:ASN:HD21	1:E:221:GLN:HE21	1.56	0.52
1:G:177:LEU:HD22	1:G:184:ILE:HD13	1.92	0.52
1:D:154:ASN:HD21	1:D:221:GLN:HE21	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:ALA:O	1:H:221:GLN:HG3	2.10	0.52
1:G:61:THR:HB	1:G:267:MET:HE2	1.90	0.52
1:D:217:ALA:O	1:D:221:GLN:HG3	2.10	0.52
1:D:177:LEU:HD22	1:D:184:ILE:HD13	1.92	0.52
1:C:128:GLU:O	1:C:131:LEU:HB2	2.10	0.52
1:G:128:GLU:O	1:G:131:LEU:HB2	2.10	0.52
1:C:71:PRO:HG2	1:C:117:SER:OG	2.08	0.52
1:F:217:ALA:O	1:F:221:GLN:HG3	2.10	0.52
1:G:217:ALA:O	1:G:221:GLN:HG3	2.10	0.52
1:C:39:ARG:HA	1:C:187:HIS:CD2	2.45	0.52
1:D:39:ARG:HA	1:D:187:HIS:CD2	2.45	0.52
1:H:128:GLU:O	1:H:131:LEU:HB2	2.10	0.52
1:H:154:ASN:HD21	1:H:221:GLN:HE21	1.56	0.52
1:B:154:ASN:HD21	1:B:221:GLN:HE21	1.56	0.52
1:C:217:ALA:O	1:C:221:GLN:HG3	2.10	0.51
1:G:39:ARG:HA	1:G:187:HIS:CD2	2.45	0.51
1:A:67:VAL:HG22	1:A:139:ILE:HB	1.90	0.51
1:E:203:LEU:HD23	1:E:203:LEU:C	2.31	0.51
1:A:203:LEU:HD23	1:A:203:LEU:C	2.31	0.51
1:D:203:LEU:C	1:D:203:LEU:HD23	2.31	0.51
1:E:39:ARG:HA	1:E:187:HIS:CD2	2.45	0.51
1:A:39:ARG:HA	1:A:187:HIS:CD2	2.45	0.51
1:B:203:LEU:C	1:B:203:LEU:HD23	2.31	0.51
1:E:217:ALA:O	1:E:221:GLN:HG3	2.10	0.51
1:B:128:GLU:O	1:B:131:LEU:HB2	2.10	0.51
1:E:128:GLU:O	1:E:131:LEU:HB2	2.10	0.51
1:A:128:GLU:O	1:A:131:LEU:HB2	2.10	0.51
1:F:203:LEU:HD23	1:F:203:LEU:C	2.31	0.51
1:G:203:LEU:C	1:G:203:LEU:HD23	2.31	0.51
1:B:217:ALA:O	1:B:221:GLN:HG3	2.10	0.51
1:B:177:LEU:HD22	1:B:184:ILE:HD13	1.92	0.51
1:H:203:LEU:HD23	1:H:203:LEU:C	2.31	0.51
1:H:142:ARG:HD3	3:H:814:HOH:O	2.11	0.51
1:F:128:GLU:O	1:F:131:LEU:HB2	2.10	0.51
1:B:72:VAL:HA	1:B:75:TRP:CE3	2.46	0.51
1:H:72:VAL:HA	1:H:75:TRP:CE3	2.46	0.51
1:C:203:LEU:C	1:C:203:LEU:HD23	2.31	0.51
1:E:177:LEU:HD22	1:E:184:ILE:HD13	1.92	0.51
1:G:72:VAL:HA	1:G:75:TRP:CE3	2.46	0.50
1:D:128:GLU:O	1:D:131:LEU:HB2	2.10	0.50
1:H:177:LEU:HD22	1:H:184:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:HD22	1:C:184:ILE:HD13	1.92	0.50
1:A:177:LEU:HD22	1:A:184:ILE:HD13	1.92	0.50
1:E:72:VAL:HA	1:E:75:TRP:CE3	2.46	0.50
1:C:72:VAL:HA	1:C:75:TRP:CE3	2.46	0.50
1:E:259:GLU:N	1:E:259:GLU:OE1	2.45	0.50
1:H:259:GLU:OE1	1:H:259:GLU:N	2.45	0.50
1:A:217:ALA:O	1:A:221:GLN:HG3	2.10	0.50
1:H:49:VAL:HG23	1:H:194:ALA:HB3	1.93	0.50
1:A:72:VAL:HA	1:A:75:TRP:CE3	2.46	0.50
1:C:58:LEU:HA	1:C:267:MET:CE	2.37	0.50
1:G:49:VAL:HG23	1:G:194:ALA:HB3	1.93	0.50
1:B:211:GLU:O	1:B:213:GLY:N	2.45	0.50
1:G:259:GLU:OE1	1:G:259:GLU:N	2.45	0.50
1:B:259:GLU:OE1	1:B:259:GLU:N	2.45	0.50
1:F:72:VAL:HA	1:F:75:TRP:CE3	2.46	0.50
1:G:58:LEU:HD23	1:G:267:MET:CE	2.41	0.50
1:A:211:GLU:O	1:A:213:GLY:N	2.45	0.50
1:E:211:GLU:O	1:E:213:GLY:N	2.45	0.50
1:F:177:LEU:HD22	1:F:184:ILE:HD13	1.92	0.49
1:A:142:ARG:HD3	3:A:313:HOH:O	2.11	0.49
1:D:72:VAL:HA	1:D:75:TRP:CE3	2.46	0.49
1:A:58:LEU:HD23	1:A:267:MET:CE	2.41	0.49
1:D:211:GLU:O	1:D:213:GLY:N	2.45	0.49
1:C:211:GLU:O	1:C:213:GLY:N	2.45	0.49
1:F:142:ARG:HD3	3:F:614:HOH:O	2.11	0.49
1:C:49:VAL:HG23	1:C:194:ALA:HB3	1.93	0.49
1:G:142:ARG:HD3	3:G:714:HOH:O	2.11	0.49
1:G:211:GLU:O	1:G:213:GLY:N	2.45	0.49
1:E:58:LEU:HD23	1:E:267:MET:CE	2.41	0.49
1:A:259:GLU:OE1	1:A:259:GLU:N	2.45	0.49
1:D:58:LEU:HD23	1:D:267:MET:CE	2.41	0.49
1:B:49:VAL:HG23	1:B:194:ALA:HB3	1.93	0.49
1:C:142:ARG:HD3	3:C:314:HOH:O	2.11	0.49
1:F:211:GLU:O	1:F:213:GLY:N	2.45	0.49
1:C:259:GLU:N	1:C:259:GLU:OE1	2.45	0.49
1:H:211:GLU:O	1:H:213:GLY:N	2.45	0.49
1:D:142:ARG:HD3	3:D:315:HOH:O	2.11	0.49
1:B:142:ARG:HD3	3:B:315:HOH:O	2.11	0.49
1:F:49:VAL:HG23	1:F:194:ALA:HB3	1.93	0.49
1:F:259:GLU:N	1:F:259:GLU:OE1	2.45	0.49
1:D:259:GLU:OE1	1:D:259:GLU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:VAL:HG23	1:E:194:ALA:HB3	1.93	0.49
1:E:164:ILE:HD12	1:F:78:ILE:HG13	1.95	0.49
1:D:49:VAL:HG23	1:D:194:ALA:HB3	1.93	0.49
1:B:58:LEU:HD23	1:B:267:MET:CE	2.41	0.48
1:G:164:ILE:HD12	1:H:78:ILE:HG13	1.94	0.48
1:A:49:VAL:HG23	1:A:194:ALA:HB3	1.93	0.48
1:E:142:ARG:HD3	3:E:514:HOH:O	2.11	0.48
1:F:200:LEU:HD22	1:F:216:LEU:HB2	1.96	0.48
1:A:200:LEU:HD11	1:A:204:TYR:CE1	2.49	0.48
1:H:45:GLY:O	1:H:142:ARG:NH1	2.47	0.48
1:D:200:LEU:HD22	1:D:216:LEU:HB2	1.96	0.48
1:D:200:LEU:HD11	1:D:204:TYR:CE1	2.49	0.48
1:B:200:LEU:HD11	1:B:204:TYR:CE1	2.49	0.48
1:D:45:GLY:O	1:D:142:ARG:NH1	2.47	0.48
1:B:200:LEU:HD22	1:B:216:LEU:HB2	1.96	0.48
1:E:200:LEU:HD11	1:E:204:TYR:CE1	2.49	0.48
1:G:200:LEU:HD22	1:G:216:LEU:HB2	1.96	0.48
1:F:200:LEU:HD11	1:F:204:TYR:CE1	2.49	0.48
1:G:45:GLY:O	1:G:142:ARG:NH1	2.47	0.48
1:C:45:GLY:O	1:C:142:ARG:NH1	2.47	0.48
1:E:45:GLY:O	1:E:142:ARG:NH1	2.47	0.47
1:A:45:GLY:O	1:A:142:ARG:NH1	2.47	0.47
1:H:200:LEU:HD11	1:H:204:TYR:CE1	2.49	0.47
1:C:200:LEU:HD11	1:C:204:TYR:CE1	2.49	0.47
1:E:200:LEU:HD22	1:E:216:LEU:HB2	1.96	0.47
1:C:200:LEU:HD22	1:C:216:LEU:HB2	1.96	0.47
1:B:45:GLY:O	1:B:142:ARG:NH1	2.47	0.47
1:F:233:LYS:HB2	1:G:232:HIS:CG	2.50	0.47
1:E:65:TRP:HH2	1:E:274:VAL:HG21	1.80	0.47
1:A:209:GLU:O	1:A:212:LYS:HG2	2.15	0.47
1:E:209:GLU:O	1:E:212:LYS:HG2	2.15	0.47
1:A:200:LEU:HD22	1:A:216:LEU:HB2	1.96	0.47
1:G:200:LEU:HD11	1:G:204:TYR:CE1	2.49	0.47
1:H:200:LEU:HD22	1:H:216:LEU:HB2	1.96	0.47
1:D:240:GLU:O	1:D:243:MET:HB2	2.15	0.47
1:F:45:GLY:O	1:F:142:ARG:NH1	2.47	0.47
1:F:92:LEU:N	3:F:624:HOH:O	2.48	0.47
1:A:164:ILE:HD12	1:B:78:ILE:HG13	1.96	0.47
1:H:209:GLU:O	1:H:212:LYS:HG2	2.15	0.47
1:F:209:GLU:O	1:F:212:LYS:HG2	2.15	0.47
1:F:240:GLU:O	1:F:243:MET:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:GLU:O	1:D:212:LYS:HG2	2.15	0.47
1:G:41:LEU:HB2	1:G:139:ILE:HD13	1.97	0.47
1:B:240:GLU:O	1:B:243:MET:HB2	2.15	0.47
1:A:78:ILE:HG13	1:B:164:ILE:HD12	1.96	0.46
1:C:209:GLU:O	1:C:212:LYS:HG2	2.15	0.46
1:C:65:TRP:HH2	1:C:274:VAL:HG21	1.80	0.46
1:G:209:GLU:O	1:G:212:LYS:HG2	2.15	0.46
1:E:41:LEU:HB2	1:E:139:ILE:HD13	1.97	0.46
1:H:41:LEU:HB2	1:H:139:ILE:HD13	1.97	0.46
1:C:240:GLU:O	1:C:243:MET:HB2	2.15	0.46
1:A:158:ASN:ND2	1:A:160:SER:H	2.14	0.46
1:H:158:ASN:ND2	1:H:160:SER:H	2.14	0.46
1:G:65:TRP:HH2	1:G:274:VAL:HG21	1.80	0.46
1:A:240:GLU:O	1:A:243:MET:HB2	2.15	0.46
1:F:158:ASN:ND2	1:F:160:SER:H	2.14	0.46
1:A:70:GLU:HB2	1:A:141:GLU:CB	2.45	0.46
1:H:240:GLU:O	1:H:243:MET:HB2	2.15	0.46
1:G:240:GLU:O	1:G:243:MET:HB2	2.15	0.46
1:H:92:LEU:N	3:H:824:HOH:O	2.48	0.46
1:B:41:LEU:HB2	1:B:139:ILE:HD13	1.97	0.46
1:G:92:LEU:N	3:G:724:HOH:O	2.48	0.46
1:B:158:ASN:ND2	1:B:160:SER:H	2.14	0.46
1:B:209:GLU:O	1:B:212:LYS:HG2	2.15	0.46
1:C:92:LEU:N	3:C:324:HOH:O	2.48	0.46
1:D:92:LEU:N	3:D:325:HOH:O	2.48	0.46
1:E:240:GLU:O	1:E:243:MET:HB2	2.15	0.46
1:G:245:ILE:HG23	1:G:246:PRO:HD2	1.98	0.46
1:D:41:LEU:HB2	1:D:139:ILE:HD13	1.97	0.46
1:C:41:LEU:HB2	1:C:139:ILE:HD13	1.97	0.46
1:F:41:LEU:HB2	1:F:139:ILE:HD13	1.97	0.46
1:B:92:LEU:N	3:B:325:HOH:O	2.48	0.46
1:B:210:GLU:H	1:B:210:GLU:CD	2.20	0.46
1:A:92:LEU:N	3:A:323:HOH:O	2.48	0.46
1:E:245:ILE:HG23	1:E:246:PRO:HD2	1.98	0.45
1:A:245:ILE:HG23	1:A:246:PRO:HD2	1.98	0.45
1:D:158:ASN:ND2	1:D:160:SER:H	2.14	0.45
1:H:70:GLU:HB2	1:H:141:GLU:CB	2.45	0.45
1:D:200:LEU:HD11	1:D:204:TYR:HE1	1.81	0.45
1:G:200:LEU:HD11	1:G:204:TYR:HE1	1.81	0.45
1:F:210:GLU:CD	1:F:210:GLU:H	2.20	0.45
1:E:158:ASN:ND2	1:E:160:SER:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ASN:ND2	1:C:160:SER:H	2.14	0.45
1:A:210:GLU:H	1:A:210:GLU:CD	2.20	0.45
1:C:210:GLU:CD	1:C:210:GLU:H	2.20	0.45
1:E:92:LEU:N	3:E:524:HOH:O	2.48	0.45
1:G:210:GLU:CD	1:G:210:GLU:H	2.20	0.45
1:E:210:GLU:CD	1:E:210:GLU:H	2.20	0.45
1:A:118:ARG:O	1:A:121:VAL:HG12	2.17	0.45
1:A:65:TRP:HH2	1:A:274:VAL:HG21	1.80	0.45
1:D:65:TRP:HH2	1:D:274:VAL:HG21	1.80	0.45
1:B:200:LEU:HD11	1:B:204:TYR:HE1	1.81	0.45
1:H:210:GLU:H	1:H:210:GLU:CD	2.20	0.45
1:F:245:ILE:HG23	1:F:246:PRO:HD2	1.98	0.45
1:H:118:ARG:O	1:H:121:VAL:HG12	2.17	0.45
1:C:70:GLU:HB2	1:C:141:GLU:CB	2.46	0.45
1:E:183:ARG:NH2	1:F:179:GLU:OE1	2.40	0.45
1:E:179:GLU:OE1	1:F:183:ARG:NH2	2.34	0.45
1:G:158:ASN:ND2	1:G:160:SER:H	2.14	0.45
1:A:41:LEU:HB2	1:A:139:ILE:HD13	1.97	0.45
1:E:118:ARG:O	1:E:121:VAL:HG12	2.17	0.45
1:B:245:ILE:HG23	1:B:246:PRO:HD2	1.98	0.45
1:G:118:ARG:O	1:G:121:VAL:HG12	2.17	0.45
1:D:245:ILE:HG23	1:D:246:PRO:HD2	1.98	0.45
1:E:200:LEU:HD11	1:E:204:TYR:HE1	1.81	0.45
1:H:200:LEU:HD11	1:H:204:TYR:HE1	1.82	0.45
1:C:245:ILE:HG23	1:C:246:PRO:HD2	1.98	0.44
1:F:70:GLU:HB2	1:F:141:GLU:CB	2.45	0.44
1:H:162:SER:OG	1:H:165:GLU:HG3	2.17	0.44
1:A:46:ASN:OD1	1:A:47:ILE:N	2.48	0.44
1:F:118:ARG:O	1:F:121:VAL:HG12	2.17	0.44
1:G:162:SER:OG	1:G:165:GLU:HG3	2.17	0.44
1:H:245:ILE:HG23	1:H:246:PRO:HD2	1.98	0.44
1:F:65:TRP:HH2	1:F:274:VAL:HG21	1.80	0.44
1:C:162:SER:OG	1:C:165:GLU:HG3	2.17	0.44
1:F:162:SER:OG	1:F:165:GLU:HG3	2.17	0.44
1:C:118:ARG:O	1:C:121:VAL:HG12	2.17	0.44
1:A:200:LEU:HD11	1:A:204:TYR:HE1	1.81	0.44
1:E:162:SER:OG	1:E:165:GLU:HG3	2.18	0.44
1:B:118:ARG:O	1:B:121:VAL:HG12	2.17	0.44
1:F:46:ASN:OD1	1:F:47:ILE:N	2.48	0.44
1:B:162:SER:OG	1:B:165:GLU:HG3	2.17	0.44
1:D:118:ARG:O	1:D:121:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:SER:OG	1:D:165:GLU:HG3	2.17	0.44
1:B:70:GLU:HA	1:B:71:PRO:HD3	1.76	0.44
1:A:162:SER:OG	1:A:165:GLU:HG3	2.17	0.44
1:D:210:GLU:H	1:D:210:GLU:CD	2.20	0.44
1:A:172:TRP:CZ2	1:B:116:LEU:HB2	2.53	0.44
1:F:72:VAL:HG21	2:F:301:DTP:O2A	2.17	0.44
1:C:46:ASN:OD1	1:C:47:ILE:N	2.48	0.44
1:A:70:GLU:HG2	3:A:321:HOH:O	2.18	0.43
1:D:70:GLU:HB2	1:D:141:GLU:CB	2.45	0.43
1:H:46:ASN:OD1	1:H:47:ILE:N	2.48	0.43
1:C:158:ASN:HD22	1:C:159:GLY:N	2.17	0.43
1:D:70:GLU:HG2	3:D:323:HOH:O	2.18	0.43
1:F:70:GLU:HG2	3:F:622:HOH:O	2.18	0.43
1:F:200:LEU:HD11	1:F:204:TYR:HE1	1.81	0.43
1:E:70:GLU:HB2	1:E:141:GLU:CB	2.45	0.43
1:G:179:GLU:OE1	1:H:183:ARG:NH2	2.39	0.43
1:D:256:PHE:CD1	1:D:256:PHE:C	2.92	0.43
1:H:58:LEU:HD23	1:H:267:MET:CE	2.41	0.43
1:D:72:VAL:HG21	2:D:301:DTP:O2A	2.19	0.43
1:H:256:PHE:C	1:H:256:PHE:CD1	2.92	0.43
1:C:70:GLU:HA	1:C:71:PRO:HD3	1.76	0.43
1:B:256:PHE:C	1:B:256:PHE:CD1	2.92	0.43
1:B:65:TRP:HH2	1:B:274:VAL:HG21	1.80	0.43
1:E:46:ASN:OD1	1:E:47:ILE:N	2.48	0.43
1:F:197:GLN:H	1:F:197:GLN:CD	2.22	0.43
1:C:256:PHE:C	1:C:256:PHE:CD1	2.92	0.43
1:E:158:ASN:HD22	1:E:159:GLY:N	2.17	0.42
1:G:70:GLU:HA	1:G:71:PRO:HD3	1.76	0.42
1:A:116:LEU:HB2	1:B:172:TRP:CZ2	2.54	0.42
1:A:197:GLN:H	1:A:197:GLN:CD	2.22	0.42
1:G:70:GLU:HG2	3:G:722:HOH:O	2.18	0.42
1:H:70:GLU:HG2	3:H:822:HOH:O	2.18	0.42
1:H:65:TRP:HH2	1:H:274:VAL:HG21	1.80	0.42
1:C:108:TYR:O	1:C:112:THR:HG23	2.20	0.42
2:H:301:DTP:H5'2	2:H:301:DTP:H2'2	1.81	0.42
1:B:158:ASN:HD22	1:B:159:GLY:N	2.17	0.42
1:G:158:ASN:HD22	1:G:159:GLY:N	2.17	0.42
1:B:70:GLU:HG2	3:B:323:HOH:O	2.18	0.42
1:D:135:LYS:HE3	1:D:275:LYS:HE2	2.02	0.42
1:G:108:TYR:O	1:G:112:THR:HG23	2.20	0.42
1:D:276:ASN:HD22	1:D:276:ASN:N	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:58:LEU:HD23	1:F:267:MET:CE	2.41	0.42
1:F:158:ASN:HD22	1:F:159:GLY:N	2.17	0.42
1:C:70:GLU:HG2	3:C:322:HOH:O	2.18	0.42
1:E:256:PHE:C	1:E:256:PHE:CD1	2.92	0.42
1:A:256:PHE:C	1:A:256:PHE:CD1	2.92	0.42
1:F:276:ASN:HD22	1:F:276:ASN:N	2.17	0.42
1:B:70:GLU:HB2	1:B:141:GLU:CB	2.45	0.42
1:C:200:LEU:HD11	1:C:204:TYR:HE1	1.82	0.42
1:B:197:GLN:H	1:B:197:GLN:CD	2.22	0.42
1:G:135:LYS:HE3	1:G:275:LYS:HE2	2.02	0.42
1:D:128:GLU:CD	1:D:128:GLU:H	2.23	0.42
1:E:108:TYR:O	1:E:112:THR:HG23	2.20	0.42
1:H:197:GLN:H	1:H:197:GLN:CD	2.22	0.42
1:G:72:VAL:HG21	2:G:301:DTP:O2A	2.20	0.42
1:A:158:ASN:HD22	1:A:159:GLY:N	2.17	0.42
1:E:70:GLU:HG2	3:E:522:HOH:O	2.18	0.42
1:E:135:LYS:HE3	1:E:275:LYS:HE2	2.02	0.42
1:F:256:PHE:CD1	1:F:256:PHE:C	2.92	0.42
1:H:108:TYR:O	1:H:112:THR:HG23	2.20	0.42
1:H:276:ASN:HD22	1:H:276:ASN:N	2.17	0.42
1:E:128:GLU:H	1:E:128:GLU:CD	2.23	0.42
1:G:128:GLU:CD	1:G:128:GLU:H	2.23	0.42
1:C:135:LYS:HE3	1:C:275:LYS:HE2	2.02	0.42
1:H:135:LYS:HE3	1:H:275:LYS:HE2	2.01	0.42
1:E:187:HIS:O	1:E:246:PRO:HD2	2.20	0.42
1:B:72:VAL:HG21	2:B:301:DTP:O2A	2.20	0.42
1:B:75:TRP:HD1	1:B:113:PHE:HE2	1.68	0.42
1:F:128:GLU:CD	1:F:128:GLU:H	2.23	0.42
1:A:75:TRP:HD1	1:A:113:PHE:HE2	1.68	0.42
1:A:108:TYR:O	1:A:112:THR:HG23	2.20	0.42
1:C:197:GLN:CD	1:C:197:GLN:H	2.22	0.42
1:G:256:PHE:CD1	1:G:256:PHE:C	2.92	0.42
1:C:276:ASN:HD22	1:C:276:ASN:N	2.17	0.42
1:D:158:ASN:HD22	1:D:159:GLY:N	2.17	0.42
1:F:108:TYR:O	1:F:112:THR:HG23	2.20	0.42
1:B:108:TYR:O	1:B:112:THR:HG23	2.20	0.42
1:H:187:HIS:O	1:H:246:PRO:HD2	2.20	0.41
1:B:187:HIS:O	1:B:246:PRO:HD2	2.20	0.41
2:G:301:DTP:H2'2	2:G:301:DTP:H5'2	1.83	0.41
1:D:75:TRP:HD1	1:D:113:PHE:HE2	1.68	0.41
1:H:128:GLU:CD	1:H:128:GLU:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:ILE:HG13	1:F:164:ILE:HD12	2.00	0.41
1:D:108:TYR:O	1:D:112:THR:HG23	2.20	0.41
1:G:46:ASN:OD1	1:G:47:ILE:N	2.48	0.41
1:D:197:GLN:H	1:D:197:GLN:CD	2.22	0.41
1:C:187:HIS:O	1:C:246:PRO:HD2	2.20	0.41
1:A:276:ASN:HD22	1:A:276:ASN:N	2.17	0.41
1:G:197:GLN:CD	1:G:197:GLN:H	2.22	0.41
1:H:158:ASN:HD22	1:H:159:GLY:N	2.17	0.41
1:F:70:GLU:HA	1:F:71:PRO:HD3	1.76	0.41
1:E:197:GLN:H	1:E:197:GLN:CD	2.22	0.41
1:G:276:ASN:N	1:G:276:ASN:HD22	2.17	0.41
1:A:135:LYS:HE3	1:A:275:LYS:HE2	2.02	0.41
1:C:128:GLU:H	1:C:128:GLU:CD	2.23	0.41
1:A:128:GLU:CD	1:A:128:GLU:H	2.23	0.41
1:F:177:LEU:HD22	1:F:184:ILE:CD1	2.51	0.41
1:F:135:LYS:HE3	1:F:275:LYS:HE2	2.02	0.41
1:E:276:ASN:N	1:E:276:ASN:HD22	2.17	0.41
1:B:124:GLU:HA	1:B:125:PRO:HD3	1.91	0.41
1:G:187:HIS:O	1:G:246:PRO:HD2	2.20	0.41
1:H:75:TRP:HD1	1:H:113:PHE:HE2	1.68	0.41
1:A:70:GLU:HA	1:A:71:PRO:HD3	1.76	0.41
1:F:187:HIS:O	1:F:246:PRO:HD2	2.20	0.41
1:B:244:ASN:ND2	1:E:134:ARG:NH2	2.68	0.41
1:G:75:TRP:HD1	1:G:113:PHE:HE2	1.68	0.41
2:B:301:DTP:H5'2	2:B:301:DTP:H2'2	1.80	0.41
1:B:46:ASN:OD1	1:B:47:ILE:N	2.48	0.41
1:C:75:TRP:HD1	1:C:113:PHE:HE2	1.68	0.41
1:H:177:LEU:HD22	1:H:184:ILE:CD1	2.51	0.41
1:D:187:HIS:O	1:D:246:PRO:HD2	2.20	0.41
1:B:128:GLU:CD	1:B:128:GLU:H	2.23	0.41
1:H:64:GLU:O	1:H:129:LYS:HE2	2.21	0.41
1:B:135:LYS:HE3	1:B:275:LYS:HE2	2.02	0.41
1:H:72:VAL:HG21	2:H:301:DTP:O2A	2.21	0.41
1:A:172:TRP:CE2	1:B:116:LEU:HB2	2.56	0.41
1:E:75:TRP:HD1	1:E:113:PHE:HE2	1.68	0.40
1:B:276:ASN:HD22	1:B:276:ASN:N	2.17	0.40
1:A:177:LEU:HD22	1:A:184:ILE:CD1	2.51	0.40
1:G:64:GLU:O	1:G:129:LYS:HE2	2.21	0.40
1:A:187:HIS:O	1:A:246:PRO:HD2	2.20	0.40
1:C:72:VAL:HG21	2:C:301:DTP:O2A	2.21	0.40
1:G:70:GLU:HB2	1:G:141:GLU:CB	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:GLU:HA	1:E:71:PRO:HD3	1.76	0.40
1:F:64:GLU:O	1:F:129:LYS:HE2	2.21	0.40
1:B:75:TRP:HD1	1:B:113:PHE:CE2	2.40	0.40
1:H:128:GLU:HA	1:H:131:LEU:CG	2.52	0.40
1:C:177:LEU:HD22	1:C:184:ILE:CD1	2.51	0.40
1:F:233:LYS:HG3	1:G:232:HIS:HB3	2.04	0.40
1:C:64:GLU:O	1:C:129:LYS:HE2	2.21	0.40
1:D:177:LEU:HD22	1:D:184:ILE:CD1	2.51	0.40
1:E:177:LEU:HD22	1:E:184:ILE:CD1	2.51	0.40
1:D:46:ASN:OD1	1:D:47:ILE:N	2.48	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:LYS:CD	1:E:240:GLU:OE1[2_756]	0.72	1.48
1:C:135:LYS:CE	1:E:240:GLU:OE1[2_756]	0.83	1.37
1:C:135:LYS:CE	1:E:240:GLU:CD[2_756]	1.09	1.11
1:F:129:LYS:CB	1:G:63:PRO:CB[1_655]	1.21	0.99
1:B:131:LEU:CD2	1:H:275:LYS:NZ[1_565]	1.48	0.72
1:C:276:ASN:OD1	1:E:185:THR:CG2[2_756]	1.74	0.46
1:C:135:LYS:CD	1:E:240:GLU:CD[2_756]	1.81	0.39
1:F:129:LYS:CD	1:G:63:PRO:O[1_655]	1.85	0.35
1:D:178:TRP:NE1	1:G:134:ARG:NH1[2_656]	1.88	0.32
1:B:123:LEU:O	1:H:134:ARG:CD[1_565]	1.89	0.31
1:C:135:LYS:CE	1:E:240:GLU:OE2[2_756]	1.91	0.29
1:A:135:LYS:NZ	1:G:240:GLU:OE2[1_565]	1.97	0.23
1:C:135:LYS:CG	1:E:240:GLU:OE1[2_756]	1.98	0.22
1:C:135:LYS:NZ	1:E:240:GLU:OE1[2_756]	2.00	0.20
1:D:178:TRP:CD1	1:G:134:ARG:NH1[2_656]	2.05	0.15
1:F:129:LYS:CG	1:G:63:PRO:CB[1_655]	2.08	0.12
1:E:101:ARG:NH2	1:G:92:LEU:CD1[2_656]	2.15	0.05
1:B:122:GLN:O	1:H:134:ARG:NH1[1_565]	2.15	0.05
1:C:135:LYS:NZ	1:E:240:GLU:CD[2_756]	2.18	0.02
1:C:276:ASN:O	1:E:182:SER:CA[2_756]	2.19	0.01

## 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	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	11	34
1	B	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	11	34
1	C	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	11	34
1	D	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	11	34
1	E	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	11	34
1	F	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	11	34
1	G	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	11	34
1	H	225/241 (93%)	203 (90%)	18 (8%)	4 (2%)	11	34
All	All	1800/1928 (93%)	1624 (90%)	144 (8%)	32 (2%)	11	34

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	207	ALA
1	B	71	PRO
1	B	207	ALA
1	C	71	PRO
1	C	207	ALA
1	D	71	PRO
1	D	207	ALA
1	E	71	PRO
1	E	207	ALA
1	F	71	PRO
1	F	207	ALA
1	G	71	PRO
1	G	207	ALA
1	H	71	PRO
1	H	207	ALA
1	A	212	LYS

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Mol	Chain	Res	Type
1	A	255	ASP
1	B	212	LYS
1	B	255	ASP
1	C	212	LYS
1	C	255	ASP
1	D	212	LYS
1	D	255	ASP
1	E	212	LYS
1	E	255	ASP
1	F	212	LYS
1	F	255	ASP
1	G	212	LYS
1	G	255	ASP
1	H	212	LYS
1	H	255	ASP

### 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	209/216 (97%)	196 (94%)	13 (6%)	23	54
1	B	209/216 (97%)	196 (94%)	13 (6%)	23	54
1	C	209/216 (97%)	196 (94%)	13 (6%)	23	54
1	D	209/216 (97%)	196 (94%)	13 (6%)	23	54
1	E	209/216 (97%)	196 (94%)	13 (6%)	23	54
1	F	209/216 (97%)	196 (94%)	13 (6%)	23	54
1	G	209/216 (97%)	196 (94%)	13 (6%)	23	54
1	H	209/216 (97%)	196 (94%)	13 (6%)	23	54
All	All	1672/1728 (97%)	1568 (94%)	104 (6%)	23	54

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

Mol	Chain	Res	Type
1	A	39	ARG
1	A	95	LEU
1	A	99	MET
1	A	111	GLN
1	A	122	GLN
1	A	144	VAL
1	A	158	ASN
1	A	171	ASP
1	A	197	GLN
1	A	208	ARG
1	A	258	GLU
1	A	259	GLU
1	A	266	LEU
1	B	39	ARG
1	B	95	LEU
1	B	99	MET
1	B	111	GLN
1	B	122	GLN
1	B	144	VAL
1	B	158	ASN
1	B	171	ASP
1	B	197	GLN
1	B	208	ARG
1	B	258	GLU
1	B	259	GLU
1	B	266	LEU
1	C	39	ARG
1	C	95	LEU
1	C	99	MET
1	C	111	GLN
1	C	122	GLN
1	C	144	VAL
1	C	158	ASN
1	C	171	ASP
1	C	197	GLN
1	C	208	ARG
1	C	258	GLU
1	C	259	GLU
1	C	266	LEU
1	D	39	ARG
1	D	95	LEU
1	D	99	MET
1	D	111	GLN

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Mol	Chain	Res	Type
1	D	122	GLN
1	D	144	VAL
1	D	158	ASN
1	D	171	ASP
1	D	197	GLN
1	D	208	ARG
1	D	258	GLU
1	D	259	GLU
1	D	266	LEU
1	E	39	ARG
1	E	95	LEU
1	E	99	MET
1	E	111	GLN
1	E	122	GLN
1	E	144	VAL
1	E	158	ASN
1	E	171	ASP
1	E	197	GLN
1	E	208	ARG
1	E	258	GLU
1	E	259	GLU
1	E	266	LEU
1	F	39	ARG
1	F	95	LEU
1	F	99	MET
1	F	111	GLN
1	F	122	GLN
1	F	144	VAL
1	F	158	ASN
1	F	171	ASP
1	F	197	GLN
1	F	208	ARG
1	F	258	GLU
1	F	259	GLU
1	F	266	LEU
1	G	39	ARG
1	G	95	LEU
1	G	99	MET
1	G	111	GLN
1	G	122	GLN
1	G	144	VAL
1	G	158	ASN

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Mol	Chain	Res	Type
1	G	171	ASP
1	G	197	GLN
1	G	208	ARG
1	G	258	GLU
1	G	259	GLU
1	G	266	LEU
1	H	39	ARG
1	H	95	LEU
1	H	99	MET
1	H	111	GLN
1	H	122	GLN
1	H	144	VAL
1	H	158	ASN
1	H	171	ASP
1	H	197	GLN
1	H	208	ARG
1	H	258	GLU
1	H	259	GLU
1	H	266	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	187	HIS
1	A	221	GLN
1	A	271	ASN
1	A	276	ASN
1	B	158	ASN
1	B	187	HIS
1	B	221	GLN
1	B	271	ASN
1	B	276	ASN
1	C	158	ASN
1	C	187	HIS
1	C	221	GLN
1	C	271	ASN
1	C	276	ASN
1	D	158	ASN
1	D	187	HIS
1	D	221	GLN
1	D	271	ASN

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Mol	Chain	Res	Type
1	D	276	ASN
1	E	158	ASN
1	E	187	HIS
1	E	221	GLN
1	E	271	ASN
1	E	276	ASN
1	F	158	ASN
1	F	187	HIS
1	F	221	GLN
1	F	271	ASN
1	F	276	ASN
1	G	158	ASN
1	G	187	HIS
1	G	221	GLN
1	G	271	ASN
1	G	276	ASN
1	H	158	ASN
1	H	187	HIS
1	H	221	GLN
1	H	271	ASN
1	H	276	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	DTP	A	301	-	24,32,32	0.98	0	32,50,50	2.27	6 (18%)
2	DTP	B	301	-	24,32,32	0.96	0	32,50,50	2.31	7 (21%)
2	DTP	C	301	-	24,32,32	0.96	1 (4%)	32,50,50	2.34	7 (21%)
2	DTP	D	301	-	24,32,32	1.04	1 (4%)	32,50,50	2.33	4 (12%)
2	DTP	E	301	-	24,32,32	1.03	1 (4%)	32,50,50	2.28	5 (15%)
2	DTP	F	301	-	24,32,32	1.00	1 (4%)	32,50,50	2.42	5 (15%)
2	DTP	G	301	-	24,32,32	1.02	1 (4%)	32,50,50	2.36	6 (18%)
2	DTP	H	301	-	24,32,32	1.01	1 (4%)	32,50,50	2.33	5 (15%)

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	DTP	A	301	-	-	0/18/34/34	0/3/3/3
2	DTP	B	301	-	-	0/18/34/34	0/3/3/3
2	DTP	C	301	-	-	0/18/34/34	0/3/3/3
2	DTP	D	301	-	-	0/18/34/34	0/3/3/3
2	DTP	E	301	-	-	0/18/34/34	0/3/3/3
2	DTP	F	301	-	-	0/18/34/34	0/3/3/3
2	DTP	G	301	-	-	0/18/34/34	0/3/3/3
2	DTP	H	301	-	-	0/18/34/34	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	DTP	C8-N7	-2.54	1.29	1.34
2	D	301	DTP	C8-N7	-2.40	1.30	1.34
2	C	301	DTP	C8-N7	-2.26	1.30	1.34
2	E	301	DTP	C8-N7	-2.18	1.30	1.34
2	H	301	DTP	C8-N7	-2.18	1.30	1.34
2	G	301	DTP	C8-N7	-2.07	1.30	1.34

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	301	DTP	N3-C2-N1	-10.86	120.58	128.89
2	G	301	DTP	N3-C2-N1	-10.58	120.79	128.89
2	H	301	DTP	N3-C2-N1	-10.50	120.86	128.89
2	D	301	DTP	N3-C2-N1	-10.46	120.89	128.89
2	C	301	DTP	N3-C2-N1	-10.33	120.98	128.89
2	B	301	DTP	N3-C2-N1	-10.24	121.06	128.89
2	A	301	DTP	N3-C2-N1	-9.85	121.35	128.89
2	E	301	DTP	N3-C2-N1	-9.84	121.36	128.89
2	E	301	DTP	C5'-C4'-C3'	-3.96	89.54	114.64
2	G	301	DTP	C5'-C4'-C3'	-3.84	90.26	114.64
2	B	301	DTP	C5'-C4'-C3'	-3.83	90.35	114.64
2	F	301	DTP	C5'-C4'-C3'	-3.79	90.60	114.64
2	A	301	DTP	C5'-C4'-C3'	-3.78	90.69	114.64
2	D	301	DTP	C5'-C4'-C3'	-3.77	90.72	114.64
2	C	301	DTP	C5'-C4'-C3'	-3.70	91.19	114.64
2	H	301	DTP	C5'-C4'-C3'	-3.68	91.28	114.64
2	B	301	DTP	C1'-N9-C4	-2.41	123.08	127.16
2	A	301	DTP	C1'-N9-C4	-2.40	123.09	127.16
2	C	301	DTP	C1'-N9-C4	-2.25	123.34	127.16
2	G	301	DTP	C4-C5-N7	-2.22	107.44	109.48
2	G	301	DTP	C1'-N9-C4	-2.07	123.65	127.16
2	B	301	DTP	C4-C5-N7	-2.07	107.58	109.48
2	C	301	DTP	C4-C5-N7	-2.02	107.62	109.48
2	C	301	DTP	O2B-PB-O3B	2.00	114.18	105.09
2	G	301	DTP	O3'-C3'-C2'	2.01	117.41	110.74
2	H	301	DTP	O4'-C1'-N9	2.04	111.26	107.72
2	F	301	DTP	O2A-PA-O3A	2.09	114.56	105.09
2	B	301	DTP	O2A-PA-O3A	2.10	114.62	105.09
2	A	301	DTP	O2B-PB-O3B	2.14	114.82	105.09
2	H	301	DTP	O3'-C3'-C2'	2.15	117.84	110.74
2	D	301	DTP	O3'-C3'-C2'	2.15	117.86	110.74
2	B	301	DTP	O3'-C3'-C2'	2.23	118.11	110.74
2	F	301	DTP	O4'-C1'-N9	2.27	111.65	107.72
2	E	301	DTP	O4'-C1'-N9	2.30	111.71	107.72
2	E	301	DTP	O3'-C3'-C2'	2.31	118.39	110.74
2	A	301	DTP	O3'-C3'-C2'	2.31	118.39	110.74
2	C	301	DTP	O3'-C3'-C2'	2.43	118.78	110.74
2	D	301	DTP	O5'-C5'-C4'	2.70	119.09	109.12
2	E	301	DTP	O5'-C5'-C4'	2.71	119.10	109.12
2	H	301	DTP	O5'-C5'-C4'	2.78	119.37	109.12
2	B	301	DTP	O5'-C5'-C4'	2.80	119.44	109.12
2	C	301	DTP	O5'-C5'-C4'	2.81	119.47	109.12
2	A	301	DTP	O5'-C5'-C4'	2.85	119.62	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	DTP	O5'-C5'-C4'	2.85	119.64	109.12
2	F	301	DTP	O5'-C5'-C4'	2.96	120.03	109.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	DTP	1	0
2	B	301	DTP	3	0
2	C	301	DTP	2	0
2	D	301	DTP	2	0
2	E	301	DTP	1	0
2	F	301	DTP	2	0
2	G	301	DTP	3	0
2	H	301	DTP	3	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	229/241 (95%)	0.16	21 (9%) 11 5	17, 39, 92, 113	0
1	B	229/241 (95%)	0.08	10 (4%) 38 26	16, 41, 85, 104	0
1	C	229/241 (95%)	0.09	14 (6%) 25 15	12, 31, 81, 95	0
1	D	229/241 (95%)	-0.02	7 (3%) 52 40	10, 29, 70, 103	0
1	E	229/241 (95%)	0.19	16 (6%) 19 11	19, 44, 91, 109	0
1	F	229/241 (95%)	0.22	17 (7%) 17 9	16, 36, 76, 120	0
1	G	229/241 (95%)	0.10	14 (6%) 25 15	19, 39, 75, 107	0
1	H	229/241 (95%)	0.28	18 (7%) 15 8	20, 46, 90, 107	0
All	All	1832/1928 (95%)	0.14	117 (6%) 23 14	10, 38, 87, 120	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	72	VAL	7.3
1	F	75	TRP	6.6
1	H	134	ARG	6.5
1	F	73	ALA	6.4
1	H	131	LEU	5.9
1	C	130	LEU	5.6
1	A	75	TRP	5.2
1	G	75	TRP	5.2
1	F	128	GLU	5.1
1	A	130	LEU	4.9
1	F	77	ASN	4.8
1	F	132	GLN	4.6
1	F	129	LYS	4.4
1	D	244	ASN	4.2
1	H	132	GLN	4.2
1	E	131	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	H	133	ALA	4.0
1	G	76	GLN	4.0
1	A	134	ARG	4.0
1	H	72	VAL	3.8
1	H	37	GLY	3.8
1	G	72	VAL	3.7
1	H	128	GLU	3.7
1	B	75	TRP	3.7
1	A	78	ILE	3.6
1	E	79	GLN	3.6
1	C	69	THR	3.6
1	C	129	LYS	3.6
1	A	132	GLN	3.6
1	F	78	ILE	3.6
1	A	77	ASN	3.5
1	F	37	GLY	3.4
1	E	75	TRP	3.4
1	E	240	GLU	3.3
1	H	79	GLN	3.3
1	A	76	GLN	3.3
1	F	74	THR	3.3
1	C	134	ARG	3.2
1	G	71	PRO	3.1
1	B	134	ARG	3.1
1	A	93	GLY	3.1
1	E	132	GLN	3.1
1	B	128	GLU	3.1
1	F	131	LEU	3.0
1	E	76	GLN	3.0
1	A	212	LYS	3.0
1	G	261	THR	3.0
1	C	132	GLN	3.0
1	F	76	GLN	3.0
1	B	131	LEU	3.0
1	A	261	THR	3.0
1	G	132	GLN	2.9
1	H	75	TRP	2.9
1	C	79	GLN	2.9
1	H	78	ILE	2.8
1	E	256	PHE	2.8
1	E	258	GLU	2.8
1	H	130	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	242	LEU	2.8
1	G	74	THR	2.7
1	F	69	THR	2.7
1	E	78	ILE	2.7
1	D	134	ARG	2.7
1	A	72	VAL	2.7
1	H	244	ASN	2.6
1	A	257	SER	2.6
1	B	79	GLN	2.6
1	G	79	GLN	2.6
1	E	134	ARG	2.6
1	A	69	THR	2.6
1	F	204	TYR	2.5
1	G	128	GLU	2.5
1	E	128	GLU	2.5
1	G	69	THR	2.5
1	D	77	ASN	2.5
1	E	259	GLU	2.5
1	F	126	PHE	2.5
1	A	79	GLN	2.5
1	E	72	VAL	2.5
1	H	277	LEU	2.4
1	D	75	TRP	2.4
1	D	261	THR	2.4
1	E	260	VAL	2.4
1	E	135	LYS	2.4
1	G	258	GLU	2.4
1	A	73	ALA	2.3
1	C	64	GLU	2.3
1	C	73	ALA	2.3
1	A	129	LYS	2.3
1	G	70	GLU	2.3
1	D	204	TYR	2.3
1	C	131	LEU	2.3
1	A	259	GLU	2.3
1	H	65	TRP	2.3
1	A	92	LEU	2.2
1	C	74	THR	2.2
1	D	76	GLN	2.2
1	C	135	LYS	2.2
1	H	268	ARG	2.2
1	B	72	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	243	MET	2.2
1	C	75	TRP	2.2
1	B	130	LEU	2.1
1	E	59	THR	2.1
1	F	79	GLN	2.1
1	H	261	THR	2.1
1	C	76	GLN	2.1
1	C	264	GLU	2.1
1	G	259	GLU	2.1
1	A	74	THR	2.1
1	B	77	ASN	2.1
1	G	268	ARG	2.1
1	A	265	ASP	2.0
1	B	135	LYS	2.0
1	H	129	LYS	2.0
1	A	70	GLU	2.0
1	F	71	PRO	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 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DTP	D	301	30/30	0.94	0.20	0.25	22,35,54,55	0
2	DTP	C	301	30/30	0.91	0.18	-0.07	22,35,54,56	0
2	DTP	B	301	30/30	0.91	0.18	-0.16	21,36,55,55	0
2	DTP	E	301	30/30	0.89	0.19	-0.27	22,36,54,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	DTP	A	301	30/30	0.89	0.18	-0.29	22,35,55,56	0
2	DTP	F	301	30/30	0.93	0.17	-0.30	22,35,54,55	0
2	DTP	H	301	30/30	0.92	0.16	-0.34	22,36,54,55	0
2	DTP	G	301	30/30	0.93	0.15	-0.63	22,36,55,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.