



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:30 PM GMT

PDB ID : 4P2V  
Title : Structure of the AI-2 processing enzyme LsrF in complex with the product of the LsrG reaction P-HPD  
Authors : Miller, S.T.; Oh, I.K.; Xavier, K.B.  
Deposited on : 2014-03-05  
Resolution : 2.51 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

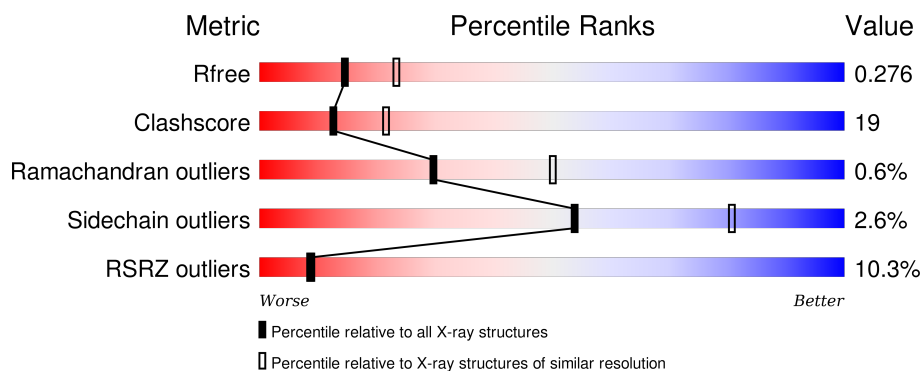
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	293	<div> <div>13%</div> <div>59%</div> <div>34%</div> <div>• •</div> </div>
1	B	293	<div> <div>2%</div> <div>70%</div> <div>25%</div> <div>•</div> </div>
1	C	293	<div> <div>10%</div> <div>66%</div> <div>29%</div> <div>• •</div> </div>
1	D	293	<div> <div>18%</div> <div>51%</div> <div>38%</div> <div>7%</div> <div>•</div> </div>
1	E	293	<div> <div>5%</div> <div>67%</div> <div>29%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	293	<div><div></div><div>2%</div><div>72%</div><div>23%</div><div></div><div></div></div>
1	G	293	<div><div></div><div>18%</div><div>59%</div><div>33%</div><div></div><div></div></div>
1	H	293	<div><div></div><div>14%</div><div>60%</div><div>35%</div><div></div><div></div></div>
1	I	293	<div><div></div><div>6%</div><div>62%</div><div>31%</div><div></div><div></div></div>
1	K	293	<div><div></div><div>9%</div><div>61%</div><div>33%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22178 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 Uncharacterized aldolase LsrF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	B	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	C	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	D	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	E	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	F	280	Total	C	N	O	S	0	0	0
			2138	1345	377	398	18			
1	G	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	H	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	I	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			
1	K	281	Total	C	N	O	S	0	0	0
			2146	1349	378	401	18			

There are 30 discrepancies between the modelled and reference sequences:

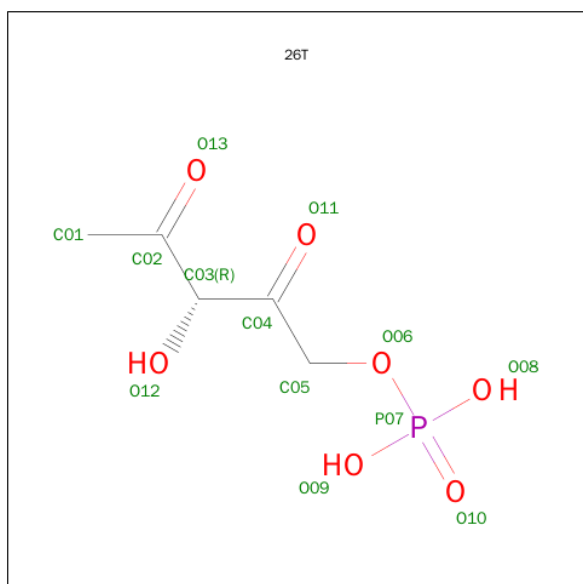
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P76143
A	0	SER	-	expression tag	UNP P76143
A	203	ALA	LYS	engineered mutation	UNP P76143
B	-1	GLY	-	expression tag	UNP P76143
B	0	SER	-	expression tag	UNP P76143
B	203	ALA	LYS	engineered mutation	UNP P76143
C	-1	GLY	-	expression tag	UNP P76143
C	0	SER	-	expression tag	UNP P76143
C	203	ALA	LYS	engineered mutation	UNP P76143

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP P76143
D	0	SER	-	expression tag	UNP P76143
D	203	ALA	LYS	engineered mutation	UNP P76143
E	-1	GLY	-	expression tag	UNP P76143
E	0	SER	-	expression tag	UNP P76143
E	203	ALA	LYS	engineered mutation	UNP P76143
F	-1	GLY	-	expression tag	UNP P76143
F	0	SER	-	expression tag	UNP P76143
F	203	ALA	LYS	engineered mutation	UNP P76143
G	-1	GLY	-	expression tag	UNP P76143
G	0	SER	-	expression tag	UNP P76143
G	203	ALA	LYS	engineered mutation	UNP P76143
H	-1	GLY	-	expression tag	UNP P76143
H	0	SER	-	expression tag	UNP P76143
H	203	ALA	LYS	engineered mutation	UNP P76143
I	-1	GLY	-	expression tag	UNP P76143
I	0	SER	-	expression tag	UNP P76143
I	203	ALA	LYS	engineered mutation	UNP P76143
K	-1	GLY	-	expression tag	UNP P76143
K	0	SER	-	expression tag	UNP P76143
K	203	ALA	LYS	engineered mutation	UNP P76143

- Molecule 2 is (3R)-3-hydroxy-2,4-dioxopentyl dihydrogen phosphate (three-letter code: 26T) (formula: C<sub>5</sub>H<sub>9</sub>O<sub>7</sub>P).

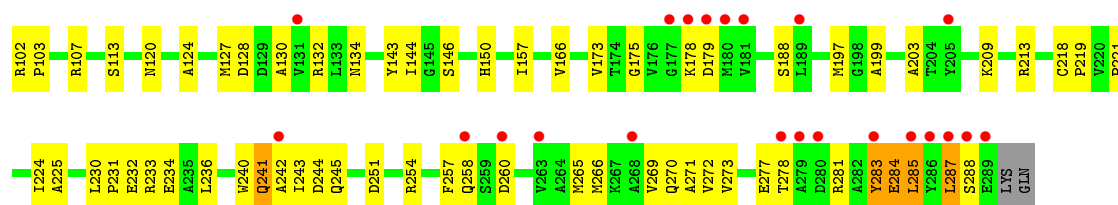


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			13	5	7	1		
2	B	1	Total	C	O	P	0	0
			13	5	7	1		
2	C	1	Total	C	O	P	0	0
			13	5	7	1		
2	D	1	Total	C	O	P	0	0
			13	5	7	1		
2	E	1	Total	C	O	P	0	0
			13	5	7	1		
2	F	1	Total	C	O	P	0	0
			13	5	7	1		
2	G	1	Total	C	O	P	0	0
			13	5	7	1		
2	H	1	Total	C	O	P	0	0
			13	5	7	1		
2	I	1	Total	C	O	P	0	0
			13	5	7	1		
2	K	1	Total	C	O	P	0	0
			13	5	7	1		

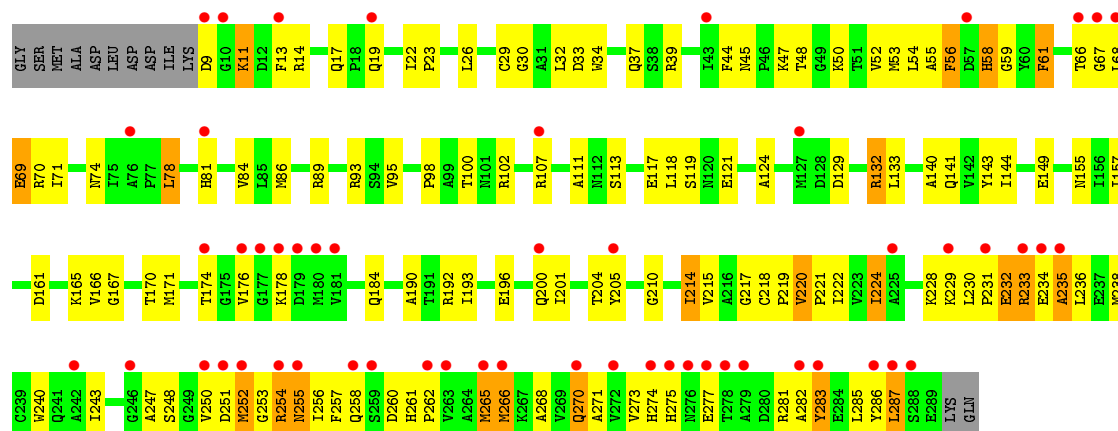
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	73	Total	O	0	0
			73	73		
3	C	66	Total	O	0	0
			66	66		
3	D	38	Total	O	0	0
			38	38		
3	E	71	Total	O	0	0
			71	71		
3	F	85	Total	O	0	0
			85	85		
3	G	47	Total	O	0	0
			47	47		
3	H	47	Total	O	0	0
			47	47		
3	I	80	Total	O	0	0
			80	80		
3	K	42	Total	O	0	0
			42	42		

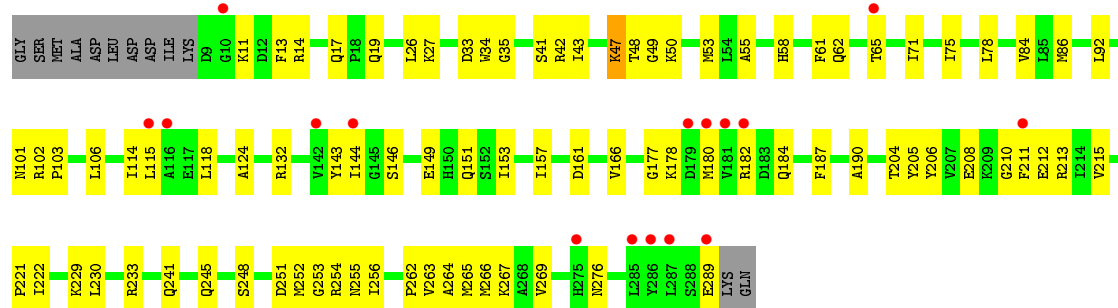




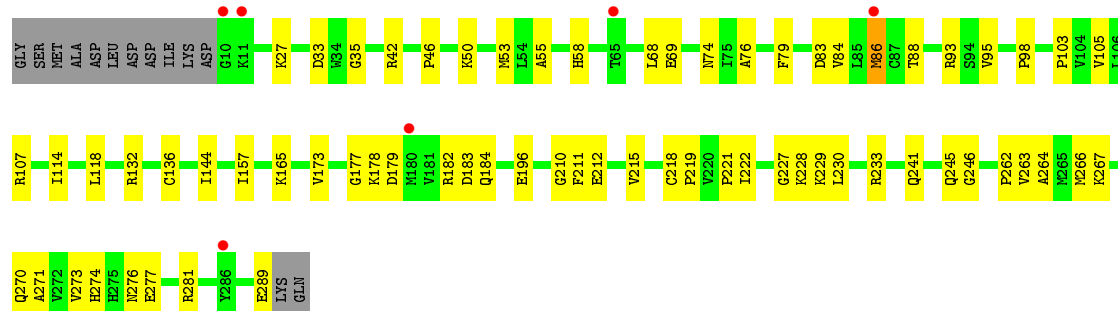
• Molecule 1: Uncharacterized aldolase LsrF



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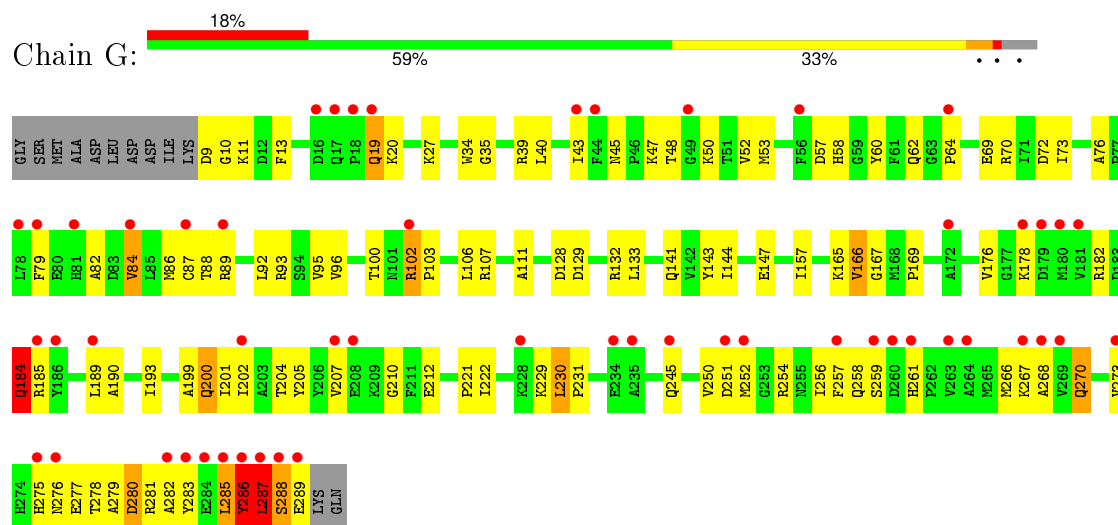


• Molecule 1: Uncharacterized aldolase LsrF

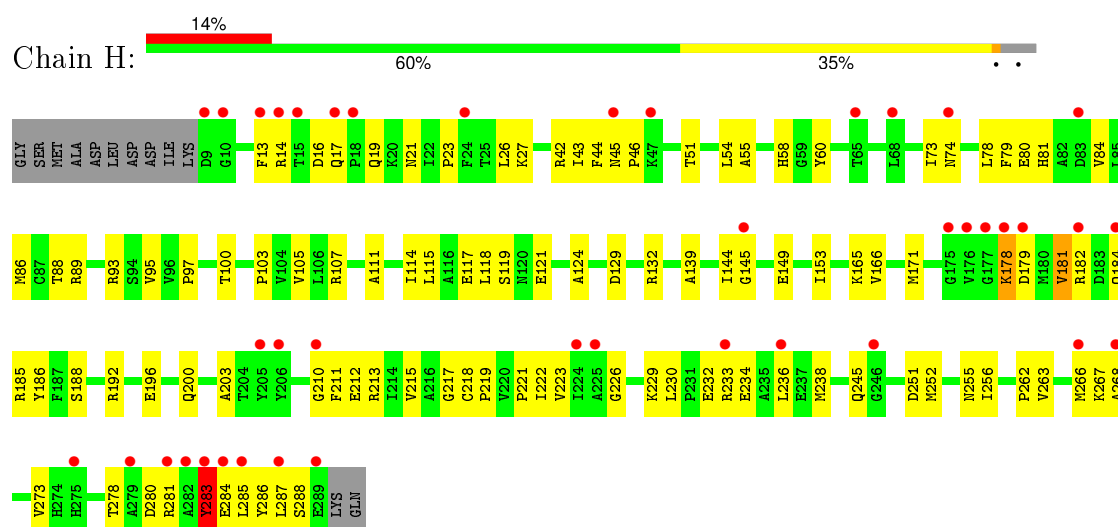




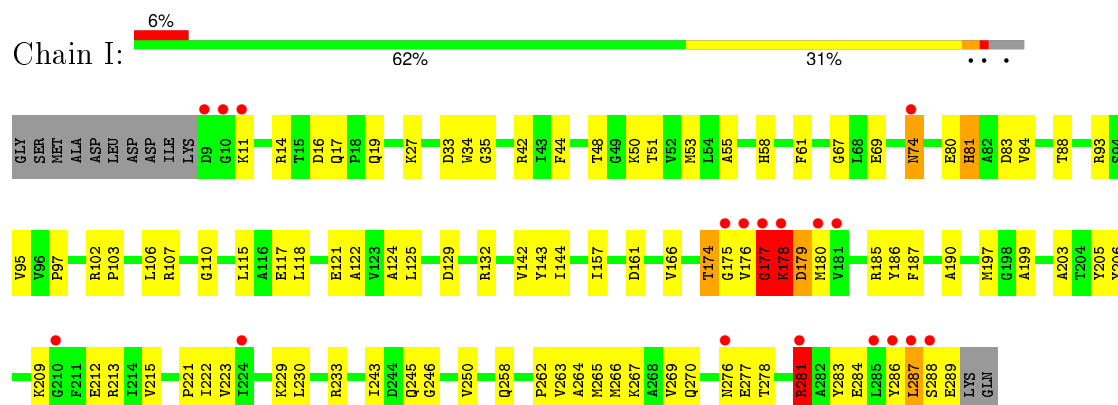
• Molecule 1: Uncharacterized aldolase LsrF



• Molecule 1: Uncharacterized aldolase LsrF

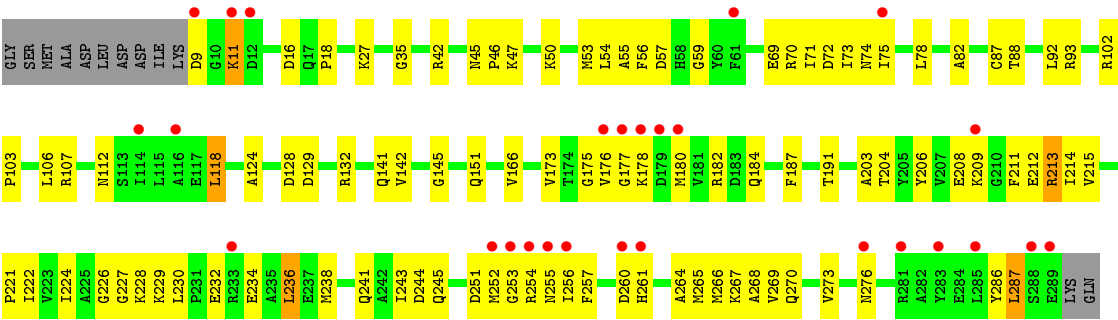


• Molecule 1: Uncharacterized aldolase LsrF



• Molecule 1: Uncharacterized aldolase LsrF





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.62Å 105.74Å 170.40Å 90.00° 101.43° 90.00°	Depositor
Resolution (Å)	49.26 – 2.51 49.26 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.26-2.51) 90.0 (49.26-2.51)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1626)	Depositor
R, $R_{free}$	0.235 , 0.271 0.237 , 0.276	Depositor DCC
$R_{free}$ test set	4585 reflections (5.21%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.6	EDS
Estimated twinning fraction	0.125 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	2 of 92513 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	22178	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 26T

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	0.37	0/2185	0.72	3/2957 (0.1%)
1	B	0.27	0/2185	0.54	0/2957
1	C	0.32	0/2185	0.67	3/2957 (0.1%)
1	D	0.43	0/2185	0.76	2/2957 (0.1%)
1	E	0.29	0/2185	0.58	0/2957
1	F	0.28	0/2177	0.55	0/2946
1	G	0.36	0/2185	0.76	3/2957 (0.1%)
1	H	0.39	1/2185 (0.0%)	0.70	0/2957
1	I	0.41	1/2185 (0.0%)	0.70	4/2957 (0.1%)
1	K	0.33	0/2185	0.73	3/2957 (0.1%)
All	All	0.35	2/21842 (0.0%)	0.68	18/29559 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	4
1	I	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	185	ARG	C-N	10.49	1.58	1.34
1	H	283	TYR	CD1-CE1	-6.17	1.30	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	287	LEU	CA-CB-CG	-10.14	91.98	115.30
1	I	281	ARG	NE-CZ-NH1	-8.64	115.98	120.30
1	K	118	LEU	CA-CB-CG	7.71	133.02	115.30
1	D	287	LEU	CA-CB-CG	-6.43	100.52	115.30
1	G	184	GLN	CA-CB-CG	6.42	127.53	113.40
1	I	281	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	G	230	LEU	CA-CB-CG	6.14	129.43	115.30
1	K	230	LEU	CA-CB-CG	6.13	129.39	115.30
1	A	16	ASP	CB-CG-OD1	5.83	123.55	118.30
1	D	232	GLU	N-CA-C	5.56	126.02	111.00
1	C	241	GLN	CA-CB-CG	-5.55	101.19	113.40
1	G	286	TYR	CA-CB-CG	5.52	123.88	113.40
1	I	179	ASP	CB-CG-OD1	5.49	123.24	118.30
1	I	177	GLY	N-CA-C	5.43	126.69	113.10
1	A	10	GLY	N-CA-C	-5.40	99.61	113.10
1	C	285	LEU	CA-CB-CG	5.35	127.61	115.30
1	A	281	ARG	CG-CD-NE	5.24	122.81	111.80
1	C	287	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	280	ASP	Peptide
1	G	285	LEU	Peptide
1	G	286	TYR	Peptide
1	G	287	LEU	Peptide
1	I	178	LYS	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2146	0	2148	98	0
1	B	2146	0	2148	61	0
1	C	2146	0	2148	76	1
1	D	2146	0	2148	182	1
1	E	2146	0	2148	69	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2138	0	2144	54	0
1	G	2146	0	2148	113	0
1	H	2146	0	2148	102	0
1	I	2146	0	2148	88	0
1	K	2146	0	2148	89	0
2	A	13	0	9	1	0
2	B	13	0	9	2	0
2	C	13	0	9	0	0
2	D	13	0	9	4	0
2	E	13	0	9	2	0
2	F	13	0	9	1	0
2	G	13	0	9	2	0
2	H	13	0	9	3	0
2	I	13	0	9	3	0
2	K	13	0	9	1	0
3	A	47	0	0	15	0
3	B	73	0	0	14	0
3	C	66	0	0	10	1
3	D	38	0	0	13	0
3	E	71	0	0	17	0
3	F	85	0	0	10	0
3	G	47	0	0	17	0
3	H	47	0	0	14	0
3	I	80	0	0	14	1
3	K	42	0	0	6	0
All	All	22178	0	21566	838	2

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 19.

All (838) 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:D:256:ILE:HG23	1:D:265:MET:SD	1.30	1.64
1:D:256:ILE:CG2	1:D:265:MET:SD	2.20	1.30
1:G:278:THR:OG1	1:G:281:ARG:CG	1.92	1.18
1:G:278:THR:OG1	1:G:281:ARG:HG2	0.99	1.15
1:B:281:ARG:NH1	3:B:402:HOH:O	1.91	1.01
1:D:23:PRO:O	3:D:416:HOH:O	1.82	0.97
1:A:141:GLN:O	3:A:413:HOH:O	1.81	0.96
1:G:268:ALA:HA	1:G:285:LEU:HD12	1.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:234:GLU:O	3:H:441:HOH:O	1.83	0.95
1:H:181:VAL:HA	1:H:182:ARG:HB2	1.52	0.92
1:D:254:ARG:HA	1:D:257:PHE:CE1	2.05	0.92
1:I:176:VAL:HG22	1:I:178:LYS:HD3	1.50	0.91
1:H:23:PRO:O	3:H:403:HOH:O	1.86	0.91
1:G:278:THR:HG1	1:G:281:ARG:HG2	1.10	0.90
1:G:169:PRO:HA	1:G:200:GLN:HE21	1.36	0.90
1:G:84:VAL:HG12	1:G:103:PRO:HB2	1.50	0.90
1:B:74:ASN:H	1:B:74:ASN:HD22	1.18	0.90
1:D:256:ILE:CD1	1:D:265:MET:HE1	2.02	0.90
1:F:196:GLU:OE2	3:F:415:HOH:O	1.88	0.89
1:G:43:ILE:HG22	1:G:84:VAL:HG11	1.55	0.89
1:D:220:VAL:HG12	1:D:221:PRO:HD2	1.55	0.88
1:B:60:TYR:O	3:B:409:HOH:O	1.91	0.88
1:G:279:ALA:O	1:G:282:ALA:HB3	1.74	0.87
1:D:66:THR:OG1	1:D:258:GLN:NE2	2.07	0.86
1:F:276:ASN:OD1	3:F:468:HOH:O	1.93	0.85
1:E:75:ILE:HD12	1:E:78:LEU:HD12	1.57	0.85
1:B:74:ASN:HD22	1:B:74:ASN:N	1.75	0.85
1:G:82:ALA:O	1:G:102:ARG:NH2	2.10	0.85
1:G:48:THR:HB	1:G:50:LYS:HE3	1.57	0.84
1:C:23:PRO:O	3:C:416:HOH:O	1.95	0.84
1:D:229:LYS:HA	1:D:255:ASN:HD22	1.43	0.84
1:G:230:LEU:HD12	1:G:231:PRO:HD2	1.60	0.83
1:D:59:GLY:O	3:D:402:HOH:O	1.95	0.83
1:K:226:GLY:O	3:K:424:HOH:O	1.96	0.83
1:D:252:MET:HE2	1:D:265:MET:HE1	1.61	0.83
1:G:276:ASN:HA	3:G:419:HOH:O	1.79	0.83
1:D:256:ILE:HG12	1:D:265:MET:CE	2.10	0.82
1:D:174:THR:HG21	1:D:190:ALA:HB1	1.62	0.82
1:D:265:MET:HG3	1:D:266:MET:N	1.95	0.81
1:D:256:ILE:HG12	1:D:265:MET:HE1	1.60	0.81
1:A:89:ARG:HD3	1:A:125:LEU:HD12	1.63	0.80
1:A:164:MET:SD	1:D:93:ARG:NH1	2.53	0.80
1:G:147:GLU:O	3:G:406:HOH:O	1.99	0.80
1:H:236:LEU:HD11	1:H:268:ALA:HB1	1.64	0.80
1:D:19:GLN:OE1	1:G:70:ARG:NH2	2.15	0.79
1:I:74:ASN:N	1:I:74:ASN:HD22	1.80	0.79
1:D:233:ARG:HD3	1:D:283:TYR:HB2	1.62	0.79
1:H:229:LYS:NZ	1:H:230:LEU:O	2.16	0.79
1:D:30:GLY:O	3:D:410:HOH:O	2.01	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:51:THR:O	3:H:443:HOH:O	1.99	0.79
1:I:80:GLU:HG3	1:I:81:HIS:ND1	1.98	0.79
1:E:161:ASP:OD2	3:E:449:HOH:O	2.00	0.78
1:G:289:GLU:OE1	3:G:401:HOH:O	2.00	0.78
1:C:11:LYS:HG2	3:C:462:HOH:O	1.84	0.78
1:D:256:ILE:CG1	1:D:265:MET:HE1	2.14	0.77
1:H:14:ARG:NH1	1:H:17:GLN:OE1	2.17	0.77
1:D:231:PRO:O	1:D:234:GLU:HG2	1.83	0.77
1:I:122:ALA:O	3:I:410:HOH:O	2.03	0.77
1:D:229:LYS:HA	1:D:255:ASN:ND2	2.00	0.76
1:D:52:VAL:O	3:D:419:HOH:O	2.02	0.76
1:E:58:HIS:NE2	3:E:469:HOH:O	2.18	0.76
1:A:177:GLY:H	1:A:180:MET:HE2	1.50	0.76
1:H:89:ARG:NH1	1:I:161:ASP:OD1	2.18	0.76
1:F:246:GLY:O	3:F:444:HOH:O	2.03	0.76
1:D:268:ALA:HA	1:D:285:LEU:HD12	1.68	0.76
1:D:107:ARG:HH12	1:D:140:ALA:HA	1.50	0.76
1:D:252:MET:HG2	1:D:256:ILE:HG13	1.68	0.75
1:D:230:LEU:HB3	1:D:234:GLU:HG3	1.67	0.75
1:E:151:GLN:OE1	3:E:456:HOH:O	2.05	0.75
1:F:271:ALA:HB1	1:F:277:GLU:HG3	1.67	0.75
1:D:254:ARG:HA	1:D:257:PHE:CZ	2.21	0.75
1:H:280:ASP:HA	1:H:283:TYR:CD1	2.21	0.75
1:F:177:GLY:O	1:F:179:ASP:N	2.18	0.74
1:A:192:ARG:NH2	3:A:406:HOH:O	2.19	0.74
1:D:14:ARG:NH1	1:D:17:GLN:OE1	2.20	0.74
1:D:271:ALA:HA	1:D:275:HIS:HB3	1.69	0.74
1:H:58:HIS:NE2	2:H:301:26T:O09	2.19	0.74
1:H:233:ARG:HA	1:H:283:TYR:CE2	2.23	0.74
1:D:58:HIS:CE1	2:D:301:26T:H5	2.23	0.74
1:D:233:ARG:CD	1:D:283:TYR:HB2	2.19	0.73
1:D:215:VAL:HG22	1:D:222:ILE:HG21	1.71	0.73
1:D:155:ASN:OD1	3:D:433:HOH:O	2.06	0.73
1:D:256:ILE:CB	1:D:265:MET:SD	2.77	0.72
1:F:212:GLU:HG2	1:F:245:GLN:HB3	1.71	0.72
1:G:88:THR:O	3:G:427:HOH:O	2.06	0.72
1:B:74:ASN:ND2	1:B:74:ASN:N	2.38	0.72
1:I:277:GLU:OE1	3:I:401:HOH:O	2.05	0.72
1:A:229:LYS:NZ	1:A:230:LEU:O	2.21	0.72
1:D:50:LYS:HA	1:D:248:SER:O	1.89	0.71
1:A:207:VAL:O	1:A:211:PHE:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:THR:HG1	1:D:258:GLN:HE21	1.38	0.71
1:C:14:ARG:NH2	3:C:436:HOH:O	2.23	0.71
1:G:87:CYS:SG	3:G:427:HOH:O	2.47	0.71
1:D:252:MET:CE	1:D:256:ILE:HG12	2.20	0.71
1:K:71:ILE:HA	1:K:75:ILE:HG22	1.71	0.71
1:H:171:MET:SD	3:H:435:HOH:O	2.47	0.71
1:G:288:SER:HB3	3:G:401:HOH:O	1.91	0.71
1:C:285:LEU:HG	1:C:288:SER:HB3	1.71	0.71
1:A:197:MET:O	3:A:439:HOH:O	2.08	0.71
1:D:224:ILE:HG22	1:D:250:VAL:HG13	1.72	0.70
1:E:41:SER:O	3:E:420:HOH:O	2.08	0.70
1:C:70:ARG:HB3	1:C:73:ILE:HB	1.73	0.70
1:D:98:PRO:O	3:D:418:HOH:O	2.07	0.70
1:H:81:HIS:HB2	1:H:266:MET:HG2	1.73	0.70
1:G:207:VAL:HG13	3:G:415:HOH:O	1.91	0.70
1:G:200:GLN:NE2	3:G:432:HOH:O	2.20	0.70
1:D:233:ARG:HD3	1:D:283:TYR:CB	2.22	0.70
1:E:213:ARG:HH22	1:K:9:ASP:HA	1.56	0.70
1:D:44:PHE:HZ	1:D:201:ILE:HD13	1.57	0.70
1:K:212:GLU:HG2	1:K:245:GLN:HB2	1.73	0.69
1:G:286:TYR:CD2	1:G:287:LEU:HA	2.26	0.69
1:B:199:ALA:O	3:B:411:HOH:O	2.09	0.69
2:E:301:26T:O10	3:E:469:HOH:O	2.09	0.69
1:B:83:ASP:OD2	1:B:274:HIS:NE2	2.25	0.69
1:D:67:GLY:O	3:D:412:HOH:O	2.09	0.69
1:E:71:ILE:O	1:E:75:ILE:HG22	1.91	0.69
1:G:212:GLU:HB3	1:G:245:GLN:HE21	1.57	0.69
1:D:100:THR:HG22	1:D:102:ARG:HG2	1.75	0.69
1:K:151:GLN:OE1	3:K:442:HOH:O	2.12	0.68
1:D:232:GLU:OE2	1:D:260:ASP:N	2.26	0.68
1:K:206:TYR:OH	1:K:208:GLU:OE1	2.08	0.68
1:B:22:ILE:O	3:B:416:HOH:O	2.12	0.68
1:K:228:LYS:HA	1:K:254:ARG:NH2	2.08	0.68
1:D:222:ILE:HG23	1:D:247:ALA:HA	1.74	0.68
1:E:208:GLU:O	3:E:450:HOH:O	2.12	0.68
1:H:81:HIS:CE1	1:H:263:VAL:HG13	2.29	0.67
1:A:117:GLU:OE1	1:A:119:SER:N	2.27	0.67
1:A:266:MET:O	1:A:270:GLN:N	2.27	0.67
1:E:62:GLN:HG2	1:E:114:ILE:HD11	1.77	0.67
1:K:264:ALA:HA	1:K:267:LYS:HG3	1.76	0.66
1:C:266:MET:O	1:C:270:GLN:HG3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:HIS:CE1	2:G:301:26T:H5	2.30	0.66
1:C:231:PRO:HD2	1:C:234:GLU:HB3	1.75	0.66
1:G:64:PRO:HG2	1:H:188:SER:HB3	1.77	0.66
1:K:187:PHE:HB3	1:K:214:ILE:HD12	1.75	0.66
1:A:125:LEU:HD21	1:A:130:ALA:HB2	1.76	0.66
1:K:228:LYS:HA	1:K:254:ARG:HH21	1.60	0.66
1:B:141:GLN:NE2	3:B:456:HOH:O	2.18	0.66
1:G:128:ASP:OD2	3:G:411:HOH:O	2.12	0.66
1:A:254:ARG:O	3:A:442:HOH:O	2.12	0.66
1:G:79:PHE:O	1:G:102:ARG:CZ	2.44	0.65
1:I:81:HIS:CD2	1:I:263:VAL:HG13	2.31	0.65
1:D:68:LEU:HD22	1:D:71:ILE:CD1	2.26	0.65
1:D:265:MET:HG3	1:D:266:MET:H	1.61	0.65
1:K:244:ASP:OD2	3:K:434:HOH:O	2.14	0.65
1:B:289:GLU:OE1	3:B:462:HOH:O	2.13	0.65
1:D:165:LYS:O	1:G:132:ARG:NH2	2.30	0.65
1:B:229:LYS:NZ	1:B:230:LEU:O	2.28	0.65
1:G:58:HIS:HE1	2:G:301:26T:H5	1.62	0.65
1:H:280:ASP:HA	1:H:283:TYR:CE1	2.30	0.64
1:D:95:VAL:HG12	1:G:19:GLN:HE21	1.62	0.64
1:C:120:ASN:OD1	3:C:450:HOH:O	2.14	0.64
1:I:143:TYR:HA	1:I:175:GLY:O	1.98	0.64
1:K:241:GLN:O	1:K:245:GLN:HG2	1.97	0.64
1:B:78:LEU:HD21	1:B:262:PRO:HB2	1.78	0.64
1:D:9:ASP:N	3:D:414:HOH:O	2.31	0.64
1:G:9:ASP:CG	1:G:10:GLY:H	2.01	0.64
1:H:117:GLU:O	3:H:429:HOH:O	2.15	0.64
1:A:212:GLU:HG2	1:A:245:GLN:HB3	1.79	0.64
1:K:191:THR:HG21	1:K:214:ILE:HD11	1.79	0.64
1:D:170:THR:OG1	3:D:406:HOH:O	2.15	0.64
1:D:144:ILE:HD12	1:D:190:ALA:HA	1.80	0.64
1:E:49:GLY:HA2	3:E:426:HOH:O	1.97	0.64
1:K:238:MET:SD	3:K:424:HOH:O	2.55	0.64
1:A:58:HIS:NE2	2:A:301:26T:O09	2.30	0.64
1:D:233:ARG:HD3	1:D:283:TYR:CG	2.33	0.63
1:H:252:MET:HG2	1:H:256:ILE:HG12	1.78	0.63
1:D:252:MET:HE3	1:D:256:ILE:HG12	1.80	0.63
1:D:17:GLN:O	1:G:70:ARG:NH1	2.31	0.63
1:D:256:ILE:CG1	1:D:265:MET:SD	2.86	0.63
1:C:124:ALA:HA	1:D:157:ILE:HD13	1.80	0.63
1:K:227:GLY:O	1:K:254:ARG:NH2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ARG:NH2	1:H:17:GLN:O	2.32	0.63
1:A:14:ARG:HG3	1:K:70:ARG:HD2	1.80	0.63
1:K:252:MET:HB3	1:K:256:ILE:HD11	1.81	0.63
1:D:11:LYS:O	1:H:213:ARG:NH2	2.32	0.63
1:A:78:LEU:HD22	1:A:266:MET:HE3	1.81	0.63
1:K:229:LYS:HA	1:K:255:ASN:OD1	1.99	0.63
1:D:262:PRO:HA	1:D:265:MET:HG2	1.81	0.63
1:K:211:PHE:HB3	1:K:245:GLN:NE2	2.13	0.63
1:I:229:LYS:NZ	1:I:230:LEU:O	2.24	0.63
1:D:174:THR:CG2	1:D:190:ALA:HB1	2.29	0.62
1:D:252:MET:HE2	1:D:265:MET:CE	2.29	0.62
1:C:240:TRP:HE3	1:C:241:GLN:HG3	1.63	0.62
1:D:11:LYS:HD3	1:H:185:ARG:HH21	1.64	0.62
1:D:204:THR:HG21	1:D:214:ILE:HD11	1.82	0.62
1:D:81:HIS:ND1	1:D:81:HIS:O	2.32	0.62
1:B:117:GLU:O	3:B:424:HOH:O	2.16	0.62
1:E:71:ILE:HG23	1:E:75:ILE:HG21	1.81	0.62
1:I:213:ARG:NH1	3:I:447:HOH:O	2.32	0.62
1:K:182:ARG:HG3	1:K:182:ARG:HH11	1.65	0.62
1:H:283:TYR:HA	1:H:286:TYR:HB3	1.82	0.62
1:D:29:CYS:O	1:D:37:GLN:NE2	2.31	0.62
1:E:263:VAL:O	1:E:267:LYS:HG2	1.99	0.61
1:B:270:GLN:HG2	1:B:274:HIS:HD2	1.65	0.61
1:E:132:ARG:O	1:F:35:GLY:HA3	2.00	0.61
1:F:136:CYS:SG	3:F:475:HOH:O	2.56	0.61
1:K:177:GLY:HA3	1:K:180:MET:HG2	1.81	0.61
1:K:27:LYS:O	1:K:221:PRO:HD3	2.01	0.61
1:D:53:MET:HB3	1:D:251:ASP:HA	1.82	0.60
1:F:183:ASP:OD2	3:F:446:HOH:O	2.16	0.60
1:I:80:GLU:HG3	1:I:81:HIS:CE1	2.36	0.60
1:K:45:ASN:OD1	1:K:47:LYS:HB2	2.01	0.60
1:E:180:MET:SD	3:E:465:HOH:O	2.57	0.60
1:A:155:ASN:OD1	3:A:432:HOH:O	2.17	0.60
1:H:184:GLN:HG3	3:H:440:HOH:O	1.99	0.60
1:I:176:VAL:HG22	1:I:178:LYS:CD	2.28	0.60
1:C:70:ARG:NE	1:H:13:PHE:O	2.32	0.60
1:F:263:VAL:HG12	1:F:267:LYS:NZ	2.16	0.60
1:H:283:TYR:HA	1:H:286:TYR:CB	2.31	0.60
1:E:27:LYS:O	1:E:221:PRO:HD3	2.01	0.60
1:A:78:LEU:HB3	1:A:266:MET:CE	2.31	0.60
1:B:33:ASP:OD2	1:I:93:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:ARG:NH1	1:G:13:PHE:O	2.28	0.60
1:B:20:LYS:HG3	3:B:404:HOH:O	2.02	0.60
1:D:254:ARG:CA	1:D:257:PHE:CZ	2.85	0.60
1:H:236:LEU:HD12	1:H:283:TYR:CE2	2.36	0.60
1:I:264:ALA:HB2	1:I:289:GLU:HB2	1.84	0.60
1:D:229:LYS:HD3	1:D:255:ASN:HA	1.84	0.59
1:C:11:LYS:HB2	1:C:13:PHE:HE1	1.66	0.59
1:H:55:ALA:HA	1:H:86:MET:HB3	1.84	0.59
1:D:34:TRP:NE1	1:G:96:VAL:O	2.26	0.59
1:C:53:MET:HB3	1:C:251:ASP:HA	1.84	0.59
1:D:89:ARG:NH1	1:D:129:ASP:OD2	2.34	0.59
1:G:199:ALA:O	3:G:444:HOH:O	2.17	0.59
1:E:92:LEU:HD22	1:E:106:LEU:HD21	1.84	0.59
1:D:95:VAL:HG12	1:G:19:GLN:NE2	2.18	0.59
1:E:252:MET:SD	1:E:255:ASN:HB2	2.42	0.59
1:B:144:ILE:HG22	1:E:115:LEU:HD12	1.85	0.59
1:I:27:LYS:O	1:I:221:PRO:HD3	2.03	0.59
1:A:144:ILE:HD12	1:A:190:ALA:HA	1.85	0.59
1:E:233:ARG:NH1	3:E:403:HOH:O	2.36	0.59
1:B:278:THR:OG1	1:B:281:ARG:HB2	2.02	0.58
1:H:233:ARG:CZ	1:H:283:TYR:HB2	2.33	0.58
1:K:107:ARG:HH12	1:K:141:GLN:HG2	1.68	0.58
1:I:278:THR:OG1	1:I:281:ARG:HB2	2.03	0.58
1:A:73:ILE:HG22	1:A:74:ASN:OD1	2.04	0.58
1:D:256:ILE:HG12	1:D:265:MET:SD	2.43	0.58
1:A:14:ARG:HD2	1:K:74:ASN:HD21	1.68	0.58
1:E:101:ASN:OD1	3:E:437:HOH:O	2.17	0.58
1:F:215:VAL:HG11	1:F:246:GLY:HA3	1.86	0.58
1:C:240:TRP:CE3	1:C:241:GLN:HG3	2.38	0.58
1:F:42:ARG:HB2	3:F:475:HOH:O	2.03	0.58
1:D:235:ALA:O	1:D:238:MET:HB3	2.04	0.58
1:I:110:GLY:N	3:I:410:HOH:O	2.14	0.58
1:D:44:PHE:CZ	1:D:201:ILE:HD13	2.38	0.58
1:G:189:LEU:O	1:G:193:ILE:HG12	2.03	0.58
1:D:235:ALA:HB1	1:D:238:MET:HB2	1.85	0.58
1:B:88:THR:HG22	1:B:107:ARG:HB3	1.86	0.58
1:A:178:LYS:HA	3:A:401:HOH:O	2.04	0.57
1:C:42:ARG:HB3	1:C:103:PRO:HG3	1.85	0.57
1:I:67:GLY:N	1:I:69:GLU:OE2	2.30	0.57
1:E:42:ARG:NH2	3:E:439:HOH:O	2.37	0.57
1:I:53:MET:HG3	1:I:84:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:MET:HE2	1:D:256:ILE:HG12	1.85	0.57
1:C:73:ILE:HG21	1:H:14:ARG:HD3	1.87	0.57
1:A:197:MET:HE3	1:D:111:ALA:H	1.70	0.57
1:D:74:ASN:ND2	3:D:429:HOH:O	2.37	0.57
1:C:281:ARG:HA	1:C:284:GLU:HG3	1.86	0.57
1:G:204:THR:HG22	1:G:205:TYR:H	1.69	0.57
1:D:261:HIS:N	1:D:262:PRO:HD3	2.19	0.57
1:C:9:ASP:N	3:C:462:HOH:O	2.37	0.57
1:B:226:GLY:HA3	3:B:452:HOH:O	2.05	0.57
1:C:128:ASP:OD1	1:C:132:ARG:NH1	2.26	0.57
1:F:27:LYS:O	1:F:221:PRO:HD3	2.05	0.57
1:G:278:THR:HG1	1:G:281:ARG:CG	1.95	0.56
1:D:174:THR:HG21	1:D:190:ALA:CB	2.33	0.56
1:D:184:GLN:HG3	1:D:210:GLY:O	2.04	0.56
1:K:57:ASP:HB3	1:K:87:CYS:HA	1.86	0.56
1:C:241:GLN:O	1:C:245:GLN:HG3	2.05	0.56
1:B:252:MET:HG2	1:B:256:ILE:HG13	1.85	0.56
1:C:88:THR:HG22	1:C:107:ARG:HB3	1.88	0.56
1:D:19:GLN:HB3	1:H:27:LYS:HD2	1.88	0.56
1:D:26:LEU:O	1:H:21:ASN:ND2	2.34	0.56
1:A:277:GLU:OE2	1:A:278:THR:N	2.39	0.56
1:G:88:THR:HG22	1:G:107:ARG:HB3	1.88	0.56
1:A:184:GLN:HE21	1:A:214:ILE:HG13	1.71	0.56
1:F:266:MET:O	1:F:270:GLN:HG2	2.05	0.56
1:K:232:GLU:O	1:K:236:LEU:HD12	2.05	0.56
1:F:277:GLU:OE1	1:F:281:ARG:HB3	2.06	0.56
1:G:144:ILE:HD13	1:G:190:ALA:HA	1.88	0.56
1:A:233:ARG:NH2	1:A:283:TYR:HB3	2.21	0.55
1:K:88:THR:HG22	1:K:107:ARG:HB3	1.87	0.55
1:D:228:LYS:HA	1:D:254:ARG:HE	1.72	0.55
1:D:270:GLN:HB2	1:D:274:HIS:NE2	2.20	0.55
1:B:124:ALA:HA	1:C:157:ILE:HD13	1.87	0.55
1:D:234:GLU:O	1:D:236:LEU:N	2.29	0.55
1:G:107:ARG:NH2	1:G:141:GLN:OE1	2.35	0.55
1:C:14:ARG:HD3	1:C:17:GLN:NE2	2.21	0.55
1:H:285:LEU:HA	1:H:288:SER:HB3	1.88	0.55
1:H:226:GLY:HA3	3:H:438:HOH:O	2.07	0.55
1:A:64:PRO:O	1:K:11:LYS:HD3	2.07	0.55
1:K:142:VAL:O	1:K:175:GLY:N	2.30	0.55
1:D:200:GLN:HA	1:D:220:VAL:HG11	1.88	0.55
1:E:11:LYS:HD3	1:E:13:PHE:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LYS:O	1:A:221:PRO:HD3	2.07	0.55
1:K:266:MET:O	1:K:270:GLN:HG2	2.06	0.55
1:D:261:HIS:ND1	1:D:287:LEU:HB3	2.22	0.54
1:D:254:ARG:CA	1:D:257:PHE:CE1	2.85	0.54
1:H:80:GLU:HG2	1:H:81:HIS:HD2	1.72	0.54
1:E:229:LYS:NZ	1:E:230:LEU:O	2.34	0.54
1:F:215:VAL:HG13	3:F:444:HOH:O	2.06	0.54
1:D:13:PHE:HB2	1:H:213:ARG:HG2	1.89	0.54
1:K:261:HIS:ND1	1:K:287:LEU:HD21	2.22	0.54
1:D:252:MET:CE	1:D:256:ILE:CG1	2.86	0.54
1:G:141:GLN:HG2	1:G:143:TYR:CZ	2.42	0.54
1:C:72:ASP:OD2	1:H:19:GLN:HG3	2.06	0.54
1:I:263:VAL:O	1:I:267:LYS:HG3	2.08	0.54
1:A:149:GLU:OE2	1:D:113:SER:HB2	2.07	0.54
1:E:184:GLN:HG3	1:E:210:GLY:O	2.08	0.54
1:A:19:GLN:HG2	1:G:27:LYS:HZ3	1.73	0.54
1:K:260:ASP:O	1:K:261:HIS:HD2	1.91	0.54
1:A:189:LEU:O	1:A:193:ILE:HD12	2.08	0.54
1:D:256:ILE:CG1	1:D:265:MET:CE	2.79	0.54
1:I:74:ASN:N	1:I:74:ASN:ND2	2.54	0.54
1:I:206:TYR:HE1	1:I:245:GLN:OE1	1.91	0.54
1:G:258:GLN:NE2	3:G:437:HOH:O	2.40	0.53
1:H:27:LYS:O	1:H:221:PRO:HD3	2.08	0.53
1:D:50:LYS:CA	1:D:248:SER:O	2.57	0.53
1:E:180:MET:O	3:E:401:HOH:O	2.19	0.53
1:F:69:GLU:OE2	3:F:429:HOH:O	2.17	0.53
1:G:254:ARG:O	1:G:258:GLN:HB3	2.08	0.53
1:H:54:LEU:N	3:H:436:HOH:O	2.42	0.53
1:A:19:GLN:HB3	1:K:70:ARG:HH12	1.74	0.53
1:I:93:ARG:NH2	1:I:129:ASP:OD1	2.42	0.53
1:H:233:ARG:HA	1:H:283:TYR:CZ	2.43	0.53
1:D:270:GLN:HB2	1:D:274:HIS:HE2	1.73	0.53
1:D:34:TRP:CE3	1:G:92:LEU:HD21	2.44	0.53
1:E:252:MET:SD	1:E:256:ILE:HG13	2.49	0.53
1:G:267:LYS:HA	1:G:270:GLN:HB2	1.90	0.53
1:G:95:VAL:O	3:G:414:HOH:O	2.18	0.53
1:I:176:VAL:CG2	1:I:186:TYR:CE2	2.92	0.53
1:H:16:ASP:OD1	1:H:17:GLN:HG3	2.09	0.53
1:D:200:GLN:NE2	3:D:427:HOH:O	2.38	0.53
1:A:69:GLU:HG2	1:K:11:LYS:HG2	1.90	0.53
1:D:256:ILE:HD13	1:D:265:MET:HE1	1.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LEU:HB2	1:D:266:MET:HE1	1.91	0.53
1:H:117:GLU:OE1	1:H:119:SER:N	2.43	0.53
1:E:101:ASN:HA	3:E:437:HOH:O	2.08	0.53
1:A:104:VAL:HG22	3:A:431:HOH:O	2.09	0.52
1:C:127:MET:HE3	1:C:130:ALA:HB3	1.91	0.52
1:A:132:ARG:O	1:K:35:GLY:HA3	2.08	0.52
1:A:9:ASP:C	1:A:11:LYS:H	2.06	0.52
1:K:82:ALA:O	1:K:102:ARG:HD3	2.09	0.52
1:I:44:PHE:HA	1:I:51:THR:OG1	2.09	0.52
1:C:224:ILE:HG22	1:C:225:ALA:O	2.09	0.52
1:K:92:LEU:HD22	1:K:106:LEU:HD21	1.91	0.52
1:K:253:GLY:N	2:K:301:26T:O08	2.29	0.52
1:I:287:LEU:O	1:I:289:GLU:N	2.42	0.52
1:E:182:ARG:HB2	1:E:187:PHE:CZ	2.44	0.52
1:A:211:PHE:HB3	1:A:245:GLN:OE1	2.10	0.52
1:A:184:GLN:NE2	1:A:213:ARG:HB2	2.24	0.52
1:H:60:TYR:OH	1:H:121:GLU:OE2	2.23	0.52
1:A:270:GLN:O	1:A:274:HIS:HB3	2.09	0.52
1:K:107:ARG:NH1	1:K:141:GLN:HG2	2.25	0.52
1:H:144:ILE:O	1:H:186:TYR:OH	2.15	0.52
1:G:202:ILE:HB	1:G:222:ILE:HG12	1.92	0.52
1:A:88:THR:HG22	1:A:107:ARG:HB3	1.92	0.52
1:D:229:LYS:NZ	1:D:232:GLU:HA	2.25	0.51
1:G:229:LYS:HG3	1:G:258:GLN:OE1	2.10	0.51
1:H:88:THR:HG22	1:H:107:ARG:HB3	1.92	0.51
1:A:157:ILE:HD13	1:D:124:ALA:HA	1.92	0.51
1:B:184:GLN:OE1	1:B:213:ARG:HD3	2.10	0.51
1:H:236:LEU:HB2	1:H:283:TYR:CZ	2.45	0.51
1:K:206:TYR:HE1	1:K:245:GLN:HE21	1.59	0.51
1:D:68:LEU:HD22	1:D:71:ILE:HD11	1.92	0.51
1:H:93:ARG:NH2	1:H:129:ASP:OD1	2.43	0.51
1:D:252:MET:CE	1:D:265:MET:CE	2.89	0.51
1:C:73:ILE:HG22	1:C:74:ASN:N	2.25	0.51
1:G:286:TYR:HD2	1:G:287:LEU:HA	1.74	0.51
1:H:184:GLN:OE1	1:H:210:GLY:HA3	2.10	0.51
1:E:53:MET:HB3	1:E:251:ASP:HA	1.93	0.51
1:I:88:THR:HG22	1:I:107:ARG:HB3	1.91	0.51
1:K:53:MET:HB3	1:K:251:ASP:HA	1.91	0.51
1:H:111:ALA:H	1:I:197:MET:HE3	1.74	0.51
1:D:243:ILE:HG13	1:D:273:VAL:HG12	1.92	0.51
1:I:287:LEU:O	1:I:289:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:THR:HG21	1:D:222:ILE:HD11	1.92	0.51
1:A:252:MET:HG2	1:A:256:ILE:HG13	1.91	0.51
1:G:27:LYS:O	1:G:221:PRO:HD3	2.10	0.51
1:F:50:LYS:HD3	1:F:273:VAL:O	2.11	0.51
1:A:55:ALA:HB2	1:A:251:ASP:OD1	2.09	0.51
1:B:92:LEU:HD22	1:B:106:LEU:HD21	1.91	0.51
1:I:144:ILE:HG13	1:I:190:ALA:HA	1.92	0.51
1:A:192:ARG:HG3	3:D:402:HOH:O	2.11	0.51
1:A:19:GLN:O	3:A:410:HOH:O	2.18	0.51
1:A:284:GLU:HG2	1:A:284:GLU:O	2.10	0.51
1:D:252:MET:HE2	1:D:256:ILE:CG1	2.41	0.50
1:I:179:ASP:O	1:I:179:ASP:OD1	2.29	0.50
1:H:124:ALA:HA	1:I:157:ILE:HD13	1.92	0.50
1:G:252:MET:HG2	1:G:256:ILE:HG13	1.92	0.50
1:B:17:GLN:OE1	3:B:453:HOH:O	2.18	0.50
1:F:55:ALA:HA	1:F:86:MET:HB3	1.93	0.50
1:F:55:ALA:HA	1:F:86:MET:CB	2.41	0.50
1:A:102:ARG:NH2	3:A:422:HOH:O	2.43	0.50
1:H:233:ARG:HD3	1:H:283:TYR:CD1	2.46	0.50
1:C:231:PRO:HD2	1:C:234:GLU:CB	2.42	0.50
1:A:267:LYS:HD2	1:A:289:GLU:OE1	2.11	0.50
1:A:182:ARG:HB2	1:A:187:PHE:CZ	2.46	0.50
1:B:64:PRO:O	1:I:11:LYS:HE2	2.10	0.50
1:K:211:PHE:HB3	1:K:245:GLN:HE21	1.75	0.50
1:K:260:ASP:O	1:K:261:HIS:CD2	2.64	0.50
1:F:76:ALA:HA	1:F:79:PHE:CE2	2.47	0.50
1:D:254:ARG:O	1:D:258:GLN:HB2	2.11	0.50
1:F:264:ALA:CB	1:F:289:GLU:HB2	2.40	0.50
1:F:264:ALA:HB2	1:F:289:GLU:HB2	1.93	0.50
1:C:254:ARG:O	1:C:258:GLN:HB2	2.11	0.50
1:C:166:VAL:O	1:H:132:ARG:HA	2.11	0.50
1:E:254:ARG:HG3	3:E:469:HOH:O	2.11	0.50
1:H:58:HIS:NE2	2:H:301:26T:H5	2.26	0.50
1:A:240:TRP:NE1	1:A:278:THR:HA	2.27	0.50
1:G:256:ILE:C	1:G:258:GLN:H	2.14	0.50
1:E:61:PHE:O	1:E:114:ILE:HG12	2.12	0.50
1:B:35:GLY:HA3	1:I:132:ARG:O	2.10	0.50
1:B:58:HIS:NE2	2:B:301:26T:H5	2.26	0.50
1:G:57:ASP:HB3	1:G:87:CYS:HA	1.93	0.50
1:I:142:VAL:O	1:I:175:GLY:N	2.44	0.50
1:C:134:ASN:O	3:C:443:HOH:O	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:LEU:HD12	1:A:288:SER:N	2.26	0.50
1:D:250:VAL:HG12	1:D:252:MET:H	1.77	0.49
1:I:121:GLU:HB3	3:I:410:HOH:O	2.11	0.49
1:B:216:ALA:HB2	3:B:468:HOH:O	2.11	0.49
1:F:215:VAL:HA	1:F:222:ILE:HD12	1.95	0.49
1:A:233:ARG:HA	1:A:283:TYR:CE1	2.47	0.49
1:K:55:ALA:HB2	1:K:251:ASP:OD1	2.12	0.49
1:A:142:VAL:HA	1:A:152:SER:HB2	1.94	0.49
1:I:284:GLU:HG2	1:I:284:GLU:O	2.12	0.49
1:C:213:ARG:NH2	3:C:458:HOH:O	2.45	0.49
1:G:53:MET:HB3	1:G:251:ASP:HA	1.94	0.49
1:C:27:LYS:O	1:C:221:PRO:HD3	2.11	0.49
1:G:62:GLN:NE2	3:G:435:HOH:O	2.46	0.49
1:I:176:VAL:HG13	1:I:178:LYS:HE3	1.95	0.49
1:D:132:ARG:HA	1:G:166:VAL:O	2.12	0.49
1:K:254:ARG:HG3	1:K:257:PHE:CZ	2.47	0.49
1:K:42:ARG:HB3	1:K:103:PRO:HG3	1.94	0.49
1:A:243:ILE:HD11	1:A:273:VAL:HG13	1.93	0.49
1:G:72:ASP:OD2	1:G:73:ILE:HG13	2.13	0.49
1:H:280:ASP:HA	1:H:283:TYR:HD1	1.75	0.49
1:K:211:PHE:CZ	1:K:224:ILE:HD11	2.47	0.49
1:A:17:GLN:OE1	1:K:73:ILE:HD13	2.12	0.49
1:C:241:GLN:HA	1:C:244:ASP:HB3	1.94	0.49
1:C:224:ILE:HD11	1:C:242:ALA:HB3	1.95	0.49
1:I:215:VAL:HG11	1:I:246:GLY:HA3	1.94	0.49
1:K:182:ARG:HG3	1:K:182:ARG:NH1	2.25	0.49
1:A:15:THR:HA	3:A:427:HOH:O	2.11	0.49
1:H:200:GLN:OE1	3:H:413:HOH:O	2.20	0.49
1:G:52:VAL:HA	1:G:250:VAL:HG22	1.94	0.49
1:D:240:TRP:CD1	1:D:277:GLU:O	2.66	0.49
1:A:93:ARG:NH2	1:A:129:ASP:OD1	2.45	0.49
1:D:277:GLU:OE2	1:D:281:ARG:HB3	2.12	0.49
1:D:256:ILE:CD1	1:D:265:MET:CE	2.84	0.48
1:I:176:VAL:HG23	1:I:186:TYR:CZ	2.47	0.48
1:G:82:ALA:N	1:G:102:ARG:HH22	2.11	0.48
1:K:175:GLY:O	3:K:428:HOH:O	2.20	0.48
1:A:12:ASP:OD2	3:A:424:HOH:O	2.20	0.48
1:F:53:MET:HG3	1:F:84:VAL:HG13	1.95	0.48
1:H:73:ILE:HG22	1:H:74:ASN:OD1	2.13	0.48
1:I:93:ARG:O	3:I:409:HOH:O	2.20	0.48
1:B:93:ARG:NH2	1:B:129:ASP:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ILE:O	1:D:248:SER:N	2.36	0.48
1:D:78:LEU:HD11	1:D:262:PRO:HB2	1.96	0.48
1:F:227:GLY:N	2:F:301:26T:O10	2.45	0.48
1:G:254:ARG:HA	1:G:257:PHE:CZ	2.48	0.48
1:D:254:ARG:HA	1:D:257:PHE:CD1	2.49	0.48
1:D:93:ARG:HE	1:D:133:LEU:HD11	1.78	0.48
1:C:132:ARG:NH2	1:H:165:LYS:O	2.47	0.48
1:B:106:LEU:HB3	1:B:125:LEU:HD21	1.96	0.48
1:B:132:ARG:O	1:I:35:GLY:HA3	2.13	0.48
1:D:117:GLU:CD	1:D:118:LEU:H	2.17	0.48
1:E:211:PHE:HB3	1:E:245:GLN:OE1	2.13	0.48
1:I:176:VAL:HG23	1:I:186:TYR:CE2	2.48	0.48
1:A:78:LEU:HB3	1:A:266:MET:HE1	1.95	0.48
1:B:103:PRO:HB3	1:B:136:CYS:SG	2.54	0.48
1:D:261:HIS:CE1	1:D:287:LEU:HB3	2.48	0.48
1:H:238:MET:N	3:H:441:HOH:O	2.04	0.48
1:I:215:VAL:HA	1:I:222:ILE:HD12	1.95	0.48
1:A:124:ALA:HA	1:E:157:ILE:HD13	1.94	0.48
1:I:177:GLY:C	1:I:178:LYS:HG2	2.35	0.48
1:I:199:ALA:O	3:I:437:HOH:O	2.20	0.48
1:I:58:HIS:NE2	2:I:301:26T:H5	2.29	0.48
1:D:215:VAL:HG22	1:D:222:ILE:HD13	1.96	0.48
1:A:184:GLN:HE22	1:A:213:ARG:HB2	1.78	0.48
1:H:55:ALA:HB2	1:H:251:ASP:OD1	2.14	0.48
1:B:98:PRO:HG3	1:I:34:TRP:CD1	2.49	0.48
1:K:54:LEU:HD21	1:K:75:ILE:HD11	1.96	0.47
1:B:144:ILE:HG13	1:B:190:ALA:HA	1.96	0.47
1:G:50:LYS:HD2	1:G:273:VAL:O	2.14	0.47
1:K:204:THR:HG21	1:K:214:ILE:HD13	1.96	0.47
1:B:241:GLN:O	1:B:245:GLN:HG3	2.14	0.47
1:A:48:THR:O	1:A:50:LYS:HD2	2.14	0.47
1:F:157:ILE:HD13	1:I:124:ALA:HA	1.96	0.47
1:K:228:LYS:HD2	1:K:229:LYS:H	1.79	0.47
1:G:89:ARG:NH1	1:G:129:ASP:OD2	2.35	0.47
1:E:143:TYR:HB3	1:E:146:SER:HB2	1.95	0.47
1:A:180:MET:HE1	3:A:408:HOH:O	2.15	0.47
1:G:92:LEU:N	3:G:427:HOH:O	2.47	0.47
1:D:13:PHE:HZ	1:H:185:ARG:NH2	2.13	0.47
1:A:213:ARG:HD2	1:G:13:PHE:CE1	2.50	0.47
1:C:33:ASP:OD1	1:H:93:ARG:NH1	2.47	0.47
1:A:182:ARG:O	3:A:428:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:LYS:NZ	3:C:435:HOH:O	2.35	0.47
1:F:218:CYS:HA	1:F:219:PRO:HD3	1.77	0.47
1:G:231:PRO:HA	3:G:437:HOH:O	2.13	0.47
1:C:254:ARG:HG3	1:C:257:PHE:CZ	2.50	0.47
1:A:269:VAL:O	1:A:273:VAL:HG23	2.14	0.47
1:K:184:GLN:HG3	1:K:213:ARG:HG3	1.96	0.47
1:C:143:TYR:HB3	1:C:146:SER:HB2	1.96	0.47
1:H:232:GLU:O	1:H:283:TYR:HE2	1.97	0.47
1:H:80:GLU:HG2	1:H:81:HIS:CD2	2.50	0.47
1:A:259:SER:N	3:A:442:HOH:O	2.47	0.47
1:E:11:LYS:HD3	1:E:13:PHE:HE1	1.80	0.47
1:H:42:ARG:HB3	1:H:103:PRO:HG3	1.96	0.47
1:C:102:ARG:NH1	3:C:424:HOH:O	2.48	0.47
1:C:232:GLU:O	1:C:236:LEU:HD13	2.15	0.47
1:D:261:HIS:N	1:D:262:PRO:CD	2.78	0.47
1:K:266:MET:O	1:K:270:GLN:N	2.31	0.47
1:D:229:LYS:HZ1	1:D:232:GLU:HA	1.79	0.47
1:D:98:PRO:HG3	1:G:34:TRP:CD1	2.50	0.47
1:E:132:ARG:NH2	1:F:165:LYS:O	2.48	0.47
1:E:33:ASP:OD1	1:F:93:ARG:NH1	2.48	0.47
1:K:71:ILE:HG23	1:K:75:ILE:CG2	2.45	0.46
1:D:11:LYS:HD3	1:H:185:ARG:NH2	2.30	0.46
1:A:80:GLU:HA	1:A:102:ARG:CZ	2.45	0.46
1:H:114:ILE:HA	1:H:118:LEU:HD21	1.97	0.46
1:B:218:CYS:HA	1:B:219:PRO:HD3	1.76	0.46
1:D:256:ILE:HA	1:D:265:MET:SD	2.56	0.46
1:K:176:VAL:HG22	1:K:177:GLY:O	2.15	0.46
1:B:57:ASP:HB3	1:B:87:CYS:HA	1.97	0.46
1:G:280:ASP:HB2	1:G:283:TYR:CD2	2.50	0.46
1:C:265:MET:O	1:C:269:VAL:HG23	2.15	0.46
1:C:132:ARG:HA	1:H:166:VAL:O	2.14	0.46
1:A:69:GLU:CG	1:K:11:LYS:HG2	2.45	0.46
1:I:117:GLU:O	3:I:449:HOH:O	2.21	0.46
1:G:157:ILE:HD13	1:K:124:ALA:HA	1.96	0.46
1:D:192:ARG:HD3	1:D:217:GLY:O	2.15	0.46
1:B:254:ARG:O	1:B:258:GLN:HB2	2.16	0.46
1:C:278:THR:HB	1:C:281:ARG:HG2	1.97	0.46
1:H:211:PHE:HD2	1:H:245:GLN:HG2	1.79	0.46
1:G:107:ARG:HA	1:G:107:ARG:HD2	1.74	0.46
1:B:132:ARG:HA	1:I:166:VAL:O	2.15	0.46
1:G:107:ARG:NH2	1:G:141:GLN:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:TRP:CD2	1:G:92:LEU:HD21	2.51	0.46
1:A:69:GLU:CD	1:A:69:GLU:H	2.17	0.46
1:H:43:ILE:HG23	1:H:84:VAL:HG21	1.98	0.46
1:F:46:PRO:O	3:F:462:HOH:O	2.20	0.46
1:I:33:ASP:OD2	3:I:415:HOH:O	2.21	0.46
1:D:265:MET:HE2	1:D:266:MET:CA	2.46	0.46
1:G:76:ALA:HA	1:G:79:PHE:CE2	2.50	0.46
1:G:19:GLN:OE1	1:G:20:LYS:N	2.49	0.46
1:K:177:GLY:HA2	1:K:178:LYS:HB2	1.97	0.46
1:G:280:ASP:CB	1:G:283:TYR:HD2	2.29	0.46
1:E:34:TRP:CD1	1:F:98:PRO:HG3	2.51	0.46
1:E:35:GLY:HA3	1:F:132:ARG:O	2.15	0.46
1:K:50:LYS:HD3	1:K:243:ILE:HD12	1.97	0.46
1:H:283:TYR:C	1:H:286:TYR:H	2.19	0.46
1:D:61:PHE:CE1	2:D:301:26T:H3	2.51	0.46
1:C:278:THR:HB	1:C:281:ARG:CG	2.46	0.46
1:E:241:GLN:O	1:E:245:GLN:HG3	2.15	0.46
1:F:83:ASP:OD2	1:F:274:HIS:NE2	2.44	0.46
1:D:229:LYS:CD	1:D:255:ASN:HA	2.46	0.46
1:D:277:GLU:HA	1:D:277:GLU:OE1	2.15	0.46
1:C:243:ILE:CD1	1:C:273:VAL:HA	2.45	0.46
1:F:233:ARG:HG3	1:F:233:ARG:O	2.14	0.46
1:G:277:GLU:OE1	1:G:277:GLU:HA	2.15	0.46
2:H:301:26T:O13	3:H:425:HOH:O	2.20	0.45
1:A:241:GLN:O	1:A:245:GLN:HG3	2.15	0.45
1:D:53:MET:HG3	1:D:84:VAL:HG13	1.98	0.45
1:D:256:ILE:HD13	1:D:265:MET:CE	2.45	0.45
1:G:276:ASN:CA	3:G:419:HOH:O	2.53	0.45
1:D:230:LEU:CB	1:D:234:GLU:HG3	2.42	0.45
1:H:139:ALA:HB2	1:H:171:MET:HE2	1.99	0.45
1:A:277:GLU:OE2	1:A:281:ARG:HD2	2.15	0.45
1:H:283:TYR:CA	1:H:286:TYR:HB3	2.45	0.45
1:E:62:GLN:OE1	1:E:65:THR:HG21	2.16	0.45
1:I:58:HIS:NE2	2:I:301:26T:O09	2.34	0.45
1:B:229:LYS:NZ	3:B:463:HOH:O	2.49	0.45
1:I:142:VAL:HG13	1:I:174:THR:HA	1.99	0.45
1:E:50:LYS:HA	1:E:248:SER:O	2.16	0.45
1:D:121:GLU:CD	1:D:143:TYR:HH	2.19	0.45
1:E:118:LEU:HD23	1:E:177:GLY:HA2	1.98	0.45
1:D:132:ARG:O	1:G:35:GLY:HA3	2.16	0.45
1:I:122:ALA:N	3:I:410:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:MET:HB2	1:D:201:ILE:HG23	1.97	0.45
1:G:39:ARG:NH1	1:G:167:GLY:O	2.49	0.45
1:I:283:TYR:O	1:I:286:TYR:HB3	2.15	0.45
1:I:265:MET:O	1:I:269:VAL:HG23	2.16	0.45
1:G:45:ASN:OD1	1:G:47:LYS:HD2	2.17	0.45
1:E:265:MET:O	1:E:269:VAL:HG23	2.16	0.45
1:E:233:ARG:NH2	3:E:402:HOH:O	2.50	0.45
1:B:64:PRO:HG2	1:C:188:SER:HB3	1.98	0.45
1:I:80:GLU:HA	1:I:102:ARG:HE	1.82	0.45
1:C:73:ILE:HG21	1:H:14:ARG:NH1	2.32	0.45
1:E:215:VAL:HA	1:E:222:ILE:HD12	1.99	0.45
1:G:92:LEU:CD2	1:G:133:LEU:HD22	2.47	0.45
1:A:240:TRP:CD1	1:A:278:THR:HA	2.52	0.45
1:B:27:LYS:O	1:B:221:PRO:HD3	2.17	0.45
1:E:212:GLU:H	1:E:212:GLU:CD	2.20	0.45
1:G:40:LEU:O	1:G:43:ILE:HG13	2.17	0.45
1:E:26:LEU:HD13	3:E:426:HOH:O	2.16	0.45
1:D:55:ALA:HB2	1:D:251:ASP:OD1	2.17	0.45
1:G:185:ARG:HH12	1:G:189:LEU:HD11	1.80	0.45
1:E:144:ILE:HD13	1:E:190:ALA:HA	1.99	0.45
1:D:45:ASN:OD1	1:D:47:LYS:HB2	2.17	0.45
1:D:54:LEU:HB2	1:D:266:MET:CE	2.47	0.44
1:D:235:ALA:HB1	1:D:238:MET:CB	2.46	0.44
1:H:88:THR:HB	3:H:417:HOH:O	2.17	0.44
1:D:121:GLU:OE2	1:D:143:TYR:OH	2.32	0.44
1:C:199:ALA:O	3:C:430:HOH:O	2.21	0.44
1:G:275:HIS:O	1:G:275:HIS:CD2	2.70	0.44
1:F:271:ALA:HB1	1:F:277:GLU:CG	2.42	0.44
1:D:270:GLN:HG3	1:D:271:ALA:N	2.32	0.44
1:F:241:GLN:O	1:F:245:GLN:HG3	2.18	0.44
1:D:55:ALA:HA	1:D:86:MET:HB3	2.00	0.44
1:G:184:GLN:OE1	1:G:184:GLN:C	2.55	0.44
1:H:215:VAL:HA	1:H:222:ILE:HD12	1.98	0.44
1:I:262:PRO:O	1:I:266:MET:HG3	2.17	0.44
1:K:268:ALA:HB2	1:K:286:TYR:HB2	1.99	0.44
1:C:230:LEU:HB3	1:C:231:PRO:HD2	1.99	0.44
1:E:166:VAL:O	1:F:132:ARG:HA	2.17	0.44
1:I:203:ALA:HA	1:I:223:VAL:O	2.17	0.44
1:I:42:ARG:NH2	3:I:480:HOH:O	2.31	0.44
1:B:143:TYR:HB3	1:B:146:SER:HB2	1.98	0.44
1:F:228:LYS:NZ	1:F:229:LYS:O	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:THR:HG22	1:F:107:ARG:HB3	2.00	0.44
1:I:61:PHE:CE2	1:I:118:LEU:HD11	2.52	0.44
1:G:184:GLN:HG3	1:G:210:GLY:HA3	1.99	0.44
1:F:86:MET:HE1	1:F:105:VAL:HG12	1.99	0.44
1:G:111:ALA:HA	1:H:153:ILE:HG21	2.00	0.44
1:F:58:HIS:HB2	1:F:68:LEU:HD12	1.99	0.44
1:G:165:LYS:HG2	1:K:128:ASP:OD2	2.18	0.44
1:D:274:HIS:CE1	1:D:275:HIS:HB2	2.53	0.44
1:C:15:THR:HG21	1:I:212:GLU:HG2	1.99	0.44
1:H:81:HIS:CE1	1:H:263:VAL:CG1	2.99	0.44
1:A:115:LEU:HD12	1:E:144:ILE:HG22	1.99	0.44
1:K:215:VAL:HA	1:K:222:ILE:HD12	1.99	0.44
1:I:276:ASN:HA	3:I:461:HOH:O	2.17	0.44
1:G:178:LYS:HD3	1:G:178:LYS:HA	1.82	0.44
1:C:60:TYR:HA	1:D:196:GLU:HG2	1.98	0.44
1:G:82:ALA:O	1:G:102:ARG:CZ	2.66	0.44
1:E:206:TYR:HE2	1:E:208:GLU:HG2	1.82	0.44
1:A:112:ASN:HB3	1:A:120:ASN:O	2.18	0.44
1:C:61:PHE:HB2	1:C:113:SER:HA	2.00	0.44
1:D:22:ILE:HA	1:D:23:PRO:HD3	1.79	0.44
1:A:230:LEU:H	1:A:255:ASN:ND2	2.15	0.44
1:H:115:LEU:HD12	1:I:144:ILE:HG22	1.99	0.44
1:I:81:HIS:ND1	1:I:81:HIS:N	2.65	0.44
1:A:266:MET:O	1:A:270:GLN:HB2	2.17	0.44
1:B:9:ASP:N	3:B:405:HOH:O	2.51	0.44
1:A:218:CYS:HA	1:A:219:PRO:HD3	1.72	0.44
1:G:184:GLN:OE1	1:G:185:ARG:N	2.51	0.43
1:B:55:ALA:HB2	1:B:251:ASP:OD1	2.17	0.43
1:B:111:ALA:O	1:C:150:HIS:ND1	2.38	0.43
1:B:264:ALA:HB2	1:B:289:GLU:HB2	1.99	0.43
1:K:45:ASN:HA	1:K:46:PRO:HD3	1.78	0.43
1:I:55:ALA:HB3	2:I:301:26T:H6	1.99	0.43
1:H:79:PHE:HB3	1:H:100:THR:HG21	2.00	0.43
1:E:102:ARG:HG3	1:E:103:PRO:HD2	1.99	0.43
1:K:112:ASN:HB2	1:K:118:LEU:HA	1.99	0.43
1:H:81:HIS:ND1	1:H:263:VAL:HG13	2.32	0.43
1:I:287:LEU:C	1:I:289:GLU:H	2.22	0.43
1:I:265:MET:HA	1:I:286:TYR:HD1	1.83	0.43
1:H:278:THR:OG1	1:H:281:ARG:NE	2.51	0.43
1:I:177:GLY:H	1:I:180:MET:HE3	1.84	0.43
1:H:229:LYS:HA	1:H:255:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:GLY:HA3	3:E:469:HOH:O	2.18	0.43
1:G:193:ILE:HD13	1:K:59:GLY:O	2.18	0.43
1:G:266:MET:O	1:G:270:GLN:N	2.37	0.43
1:A:166:VAL:O	1:K:132:ARG:HA	2.17	0.43
1:E:264:ALA:HB2	1:E:289:GLU:HB2	1.99	0.43
1:C:269:VAL:O	1:C:273:VAL:HG23	2.18	0.43
1:H:281:ARG:HA	1:H:284:GLU:CB	2.48	0.43
1:D:218:CYS:HA	1:D:219:PRO:HD3	1.69	0.43
1:H:192:ARG:NE	1:H:217:GLY:O	2.51	0.43
1:D:166:VAL:O	1:G:132:ARG:HA	2.18	0.43
1:I:14:ARG:HG3	1:I:16:ASP:OD1	2.18	0.43
1:C:89:ARG:NH2	1:D:161:ASP:OD1	2.47	0.43
1:H:78:LEU:HD21	1:H:262:PRO:HB2	2.00	0.43
1:D:265:MET:HE2	1:D:266:MET:HA	2.01	0.43
1:F:211:PHE:HB3	1:F:245:GLN:OE1	2.18	0.43
1:A:16:ASP:OD1	1:A:17:GLN:HG3	2.18	0.43
1:G:204:THR:HG22	1:G:205:TYR:N	2.34	0.43
1:F:262:PRO:O	1:F:266:MET:HG3	2.18	0.43
1:D:176:VAL:HG23	1:D:205:TYR:CE2	2.53	0.43
1:K:93:ARG:NH2	1:K:129:ASP:OD1	2.52	0.43
1:H:45:ASN:OD1	1:H:46:PRO:HD2	2.19	0.43
1:H:273:VAL:HG21	3:H:443:HOH:O	2.18	0.43
1:C:11:LYS:HB2	1:C:13:PHE:CE1	2.50	0.43
1:H:184:GLN:H	1:H:184:GLN:HG3	1.55	0.43
1:K:50:LYS:HD2	1:K:273:VAL:O	2.19	0.43
1:K:70:ARG:CD	1:K:73:ILE:HD12	2.49	0.43
1:B:33:ASP:HB2	1:F:33:ASP:HB2	2.01	0.43
1:C:224:ILE:O	1:C:251:ASP:N	2.32	0.43
1:I:206:TYR:CE1	1:I:245:GLN:OE1	2.71	0.43
1:E:43:ILE:HG23	1:E:84:VAL:HG11	2.01	0.43
1:B:157:ILE:HD13	1:E:124:ALA:HA	2.01	0.43
1:F:50:LYS:NZ	3:F:427:HOH:O	2.36	0.43
1:I:243:ILE:HG21	3:I:461:HOH:O	2.19	0.43
1:C:173:VAL:HG22	1:C:203:ALA:HB3	2.01	0.43
1:G:201:ILE:HD12	3:G:429:HOH:O	2.19	0.43
1:I:177:GLY:HA3	1:I:178:LYS:HA	1.75	0.42
1:G:79:PHE:O	1:G:102:ARG:NH2	2.52	0.42
1:I:263:VAL:HG12	1:I:267:LYS:HE3	2.00	0.42
1:K:182:ARG:HB3	1:K:187:PHE:CZ	2.53	0.42
1:F:114:ILE:HA	1:F:118:LEU:HD11	2.00	0.42
1:A:61:PHE:HB2	1:A:113:SER:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:ASP:N	1:K:72:ASP:OD1	2.50	0.42
1:A:92:LEU:HD22	1:A:106:LEU:HD21	2.00	0.42
1:E:14:ARG:NH1	1:F:74:ASN:HD21	2.16	0.42
1:K:16:ASP:O	1:K:18:PRO:HD3	2.19	0.42
1:G:258:GLN:CG	1:G:259:SER:N	2.83	0.42
1:E:58:HIS:NE2	2:E:301:26T:H5	2.35	0.42
1:K:206:TYR:HB2	1:K:224:ILE:HD12	2.01	0.42
1:I:48:THR:HB	1:I:50:LYS:HE3	2.02	0.42
1:D:33:ASP:OD1	3:D:420:HOH:O	2.21	0.42
1:E:262:PRO:O	1:E:266:MET:HG3	2.19	0.42
1:H:218:CYS:HA	1:H:219:PRO:HD3	1.82	0.42
1:K:229:LYS:HE3	3:K:403:HOH:O	2.19	0.42
1:F:229:LYS:NZ	1:F:230:LEU:O	2.37	0.42
1:C:233:ARG:HB2	1:C:283:TYR:CE1	2.54	0.42
1:D:265:MET:O	1:D:268:ALA:HB3	2.20	0.42
1:D:253:GLY:HA3	2:D:301:26T:O09	2.19	0.42
1:A:256:ILE:HD13	1:A:266:MET:HG2	2.00	0.42
1:A:235:ALA:HA	1:A:238:MET:HE3	2.01	0.42
1:A:76:ALA:HA	1:A:79:PHE:CE2	2.53	0.42
1:I:106:LEU:HB3	1:I:125:LEU:HD21	2.01	0.42
1:B:115:LEU:HD12	1:C:144:ILE:HG22	2.01	0.42
1:D:262:PRO:O	1:D:265:MET:HG2	2.19	0.42
1:D:58:HIS:CE1	2:D:301:26T:C05	2.99	0.42
1:K:261:HIS:ND1	1:K:287:LEU:HD11	2.34	0.42
1:C:269:VAL:O	1:C:272:VAL:HG12	2.19	0.42
1:D:256:ILE:HD13	1:D:266:MET:HG3	2.02	0.42
1:D:273:VAL:HG23	1:D:274:HIS:N	2.35	0.42
1:F:103:PRO:HB3	1:F:136:CYS:SG	2.60	0.42
1:B:165:LYS:O	1:I:132:ARG:NH2	2.53	0.42
1:E:204:THR:CG2	1:E:205:TYR:N	2.82	0.42
1:D:250:VAL:HG12	1:D:252:MET:N	2.34	0.42
1:I:229:LYS:HB2	1:I:258:GLN:OE1	2.20	0.42
1:I:106:LEU:HG	3:I:458:HOH:O	2.19	0.42
1:D:283:TYR:HA	1:D:283:TYR:HD1	1.71	0.42
1:H:211:PHE:HB3	1:H:245:GLN:HE21	1.83	0.42
1:C:233:ARG:HB2	1:C:283:TYR:HE1	1.84	0.42
1:B:73:ILE:HD13	1:I:17:GLN:OE1	2.20	0.42
1:B:271:ALA:HA	1:B:275:HIS:HB2	2.00	0.42
1:A:53:MET:HA	1:A:84:VAL:HG13	2.02	0.42
1:C:209:LYS:HA	1:C:209:LYS:HD2	1.83	0.42
1:G:106:LEU:HA	1:G:106:LEU:HD23	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:O	1:B:224:ILE:HA	2.20	0.42
1:K:265:MET:O	1:K:269:VAL:HG23	2.19	0.42
1:B:111:ALA:H	1:C:197:MET:HE3	1.85	0.42
1:G:176:VAL:HG21	1:G:182:ARG:CZ	2.50	0.42
1:C:45:ASN:HA	1:C:46:PRO:HD3	1.94	0.42
1:H:26:LEU:HD21	1:H:44:PHE:CD2	2.54	0.42
1:C:22:ILE:HA	1:C:23:PRO:HD3	1.80	0.41
1:D:50:LYS:NZ	1:D:273:VAL:O	2.51	0.41
1:G:93:ARG:CZ	1:G:133:LEU:HD21	2.50	0.41
1:A:131:VAL:CG2	1:A:166:VAL:HG11	2.50	0.41
1:A:260:ASP:OD1	1:A:260:ASP:N	2.48	0.41
1:C:271:ALA:HB1	1:C:277:GLU:HG3	2.01	0.41
1:D:256:ILE:CA	1:D:265:MET:SD	3.08	0.41
1:D:133:LEU:CD2	1:G:34:TRP:HB3	2.49	0.41
1:A:252:MET:SD	1:A:255:ASN:HB2	2.59	0.41
1:D:67:GLY:H	1:D:69:GLU:CD	2.20	0.41
1:C:224:ILE:HD11	1:C:242:ALA:CB	2.50	0.41
1:A:260:ASP:O	1:A:261:HIS:ND1	2.54	0.41
1:H:236:LEU:HB2	1:H:283:TYR:CE2	2.56	0.41
1:H:236:LEU:HD12	1:H:283:TYR:CD2	2.55	0.41
1:E:62:GLN:HA	1:E:114:ILE:HG12	2.02	0.41
1:D:32:LEU:HB2	1:D:37:GLN:HG3	2.01	0.41
1:K:177:GLY:HA3	1:K:180:MET:CG	2.48	0.41
1:K:78:LEU:HB3	1:K:266:MET:HE3	2.02	0.41
1:D:143:TYR:O	1:D:149:GLU:HB2	2.20	0.41
1:H:281:ARG:HA	1:H:284:GLU:HB3	2.02	0.41
1:E:149:GLU:O	1:E:153:ILE:HG13	2.21	0.41
1:H:287:LEU:HG	1:H:287:LEU:O	2.20	0.41
1:G:100:THR:HG22	1:G:102:ARG:HB2	2.01	0.41
1:K:145:GLY:O	1:K:180:MET:HE1	2.19	0.41
1:G:11:LYS:HB3	1:G:13:PHE:CE1	2.56	0.41
1:A:173:VAL:HG22	1:A:203:ALA:HB3	2.02	0.41
1:C:178:LYS:O	1:C:178:LYS:HG3	2.20	0.41
1:G:278:THR:HG21	1:G:281:ARG:CZ	2.50	0.41
1:C:17:GLN:NE2	1:H:73:ILE:HD13	2.35	0.41
1:B:70:ARG:HH21	1:I:19:GLN:HG2	1.85	0.41
1:G:60:TYR:HA	1:H:196:GLU:HG2	2.02	0.41
1:D:107:ARG:HH21	1:D:141:GLN:NE2	2.18	0.41
1:I:83:ASP:O	1:I:103:PRO:HD2	2.21	0.41
1:E:55:ALA:HA	1:E:86:MET:HB3	2.02	0.41
1:C:143:TYR:CD1	1:C:175:GLY:HA3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:84:VAL:HG11	1:H:105:VAL:HG23	2.03	0.41
1:I:187:PHE:CZ	1:I:205:TYR:HB2	2.55	0.41
1:E:53:MET:HG3	1:E:84:VAL:HG13	2.03	0.41
1:I:95:VAL:O	1:I:97:PRO:HD3	2.20	0.41
1:D:144:ILE:HD13	1:D:193:ILE:HD12	2.03	0.41
1:D:133:LEU:HA	1:G:35:GLY:HA3	2.02	0.41
1:H:203:ALA:HA	1:H:223:VAL:O	2.20	0.41
1:H:203:ALA:HB2	3:H:435:HOH:O	2.20	0.41
1:A:13:PHE:CE1	1:A:15:THR:HB	2.55	0.41
1:D:13:PHE:CG	1:H:213:ARG:HG2	2.55	0.41
1:A:233:ARG:HA	1:A:283:TYR:CZ	2.56	0.41
1:G:176:VAL:HG21	1:G:182:ARG:NH1	2.36	0.41
1:B:265:MET:O	1:B:269:VAL:HG23	2.20	0.41
1:H:145:GLY:N	1:H:149:GLU:OE1	2.37	0.41
1:F:184:GLN:HG3	1:F:210:GLY:O	2.21	0.41
1:E:19:GLN:NE2	1:F:95:VAL:HG12	2.36	0.41
1:K:173:VAL:HG22	1:K:203:ALA:HB3	2.02	0.41
1:A:160:VAL:O	1:A:164:MET:HG2	2.21	0.41
1:F:212:GLU:CG	1:F:245:GLN:HB3	2.45	0.41
1:G:86:MET:HE1	1:G:107:ARG:HH11	1.86	0.41
1:D:171:MET:CB	1:D:201:ILE:HG23	2.50	0.41
1:A:12:ASP:O	1:K:69:GLU:HG3	2.21	0.41
1:D:107:ARG:HD2	1:D:107:ARG:HA	1.81	0.40
1:K:287:LEU:HA	1:K:287:LEU:HD23	1.58	0.40
1:A:132:ARG:HA	1:K:166:VAL:O	2.22	0.40
1:D:119:SER:HA	1:D:143:TYR:CZ	2.56	0.40
1:C:58:HIS:HB2	1:C:68:LEU:HD22	2.04	0.40
1:E:71:ILE:HG23	1:E:75:ILE:CG2	2.51	0.40
1:A:14:ARG:NH1	1:K:74:ASN:OD1	2.54	0.40
1:B:42:ARG:HB3	1:B:103:PRO:HG3	2.03	0.40
1:B:23:PRO:O	3:B:443:HOH:O	2.22	0.40
1:D:56:PHE:N	1:D:56:PHE:CD1	2.90	0.40
1:D:265:MET:CG	1:D:266:MET:N	2.77	0.40
3:A:427:HOH:O	1:K:70:ARG:NH2	2.53	0.40
1:B:58:HIS:HE2	2:B:301:26T:H5	1.86	0.40
1:H:95:VAL:O	1:H:97:PRO:HD3	2.22	0.40
1:E:47:LYS:HG3	1:E:48:THR:N	2.33	0.40
1:G:259:SER:HB3	1:G:261:HIS:H	1.86	0.40
1:D:236:LEU:HD12	1:D:282:ALA:HB1	2.03	0.40
1:D:48:THR:HG22	1:D:50:LYS:H	1.86	0.40
1:D:13:PHE:CE1	1:G:69:GLU:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLN:HE22	1:A:213:ARG:CB	2.34	0.40
1:G:280:ASP:N	1:G:280:ASP:OD1	2.54	0.40
1:I:265:MET:HB2	1:I:286:TYR:HE1	1.87	0.40
1:F:144:ILE:HG22	1:I:115:LEU:HD12	2.04	0.40
1:K:56:PHE:N	1:K:56:PHE:CD1	2.89	0.40
1:D:252:MET:CE	1:D:265:MET:HE3	2.51	0.40
1:E:206:TYR:CE2	1:E:208:GLU:HG2	2.56	0.40
1:C:218:CYS:HA	1:C:219:PRO:HD3	1.78	0.40
1:D:39:ARG:NH1	1:D:167:GLY:O	2.55	0.40
1:I:270:GLN:HE21	1:I:270:GLN:HB2	1.75	0.40

All (2) 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:287:LEU:O	1:D:47:LYS:NZ[2_454]	2.12	0.08
3:C:401:HOH:O	3:I:403:HOH:O[1_455]	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	279/293 (95%)	267 (96%)	12 (4%)	0	100	100
1	B	279/293 (95%)	269 (96%)	9 (3%)	1 (0%)	39	61
1	C	279/293 (95%)	266 (95%)	11 (4%)	2 (1%)	26	46
1	D	279/293 (95%)	267 (96%)	8 (3%)	4 (1%)	14	24
1	E	279/293 (95%)	268 (96%)	10 (4%)	1 (0%)	39	61
1	F	278/293 (95%)	266 (96%)	11 (4%)	1 (0%)	39	61
1	G	279/293 (95%)	266 (95%)	11 (4%)	2 (1%)	26	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	279/293 (95%)	265 (95%)	11 (4%)	3 (1%)	17	31
1	I	279/293 (95%)	265 (95%)	10 (4%)	4 (1%)	14	24
1	K	279/293 (95%)	267 (96%)	12 (4%)	0	100	100
All	All	2789/2930 (95%)	2666 (96%)	105 (4%)	18 (1%)	30	50

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	178	LYS
1	D	178	LYS
1	D	286	TYR
1	E	178	LYS
1	F	178	LYS
1	G	287	LEU
1	G	288	SER
1	C	179	ASP
1	H	178	LYS
1	H	181	VAL
1	I	177	GLY
1	I	288	SER
1	C	284	GLU
1	H	179	ASP
1	D	254	ARG
1	I	174	THR
1	I	287	LEU
1	D	235	ALA

### 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	227/237 (96%)	222 (98%)	5 (2%)	60	84
1	B	227/237 (96%)	224 (99%)	3 (1%)	76	92
1	C	227/237 (96%)	224 (99%)	3 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	227/237 (96%)	210 (92%)	17 (8%)	17	31
1	E	227/237 (96%)	224 (99%)	3 (1%)	76	92
1	F	226/237 (95%)	223 (99%)	3 (1%)	76	92
1	G	227/237 (96%)	219 (96%)	8 (4%)	43	70
1	H	227/237 (96%)	223 (98%)	4 (2%)	66	88
1	I	227/237 (96%)	220 (97%)	7 (3%)	47	75
1	K	227/237 (96%)	221 (97%)	6 (3%)	54	81
All	All	2269/2370 (96%)	2210 (97%)	59 (3%)	54	81

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	61	PHE
1	A	125	LEU
1	A	233	ARG
1	A	274	HIS
1	B	74	ASN
1	B	180	MET
1	B	285	LEU
1	C	75	ILE
1	C	260	ASP
1	C	283	TYR
1	D	11	LYS
1	D	56	PHE
1	D	58	HIS
1	D	61	PHE
1	D	69	GLU
1	D	78	LEU
1	D	132	ARG
1	D	214	ILE
1	D	220	VAL
1	D	224	ILE
1	D	233	ARG
1	D	252	MET
1	D	255	ASN
1	D	265	MET
1	D	266	MET
1	D	270	GLN
1	D	283	TYR

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Mol	Chain	Res	Type
1	E	17	GLN
1	E	47	LYS
1	E	276	ASN
1	F	86	MET
1	F	173	VAL
1	F	182	ARG
1	G	19	GLN
1	G	84	VAL
1	G	102	ARG
1	G	166	VAL
1	G	184	GLN
1	G	200	GLN
1	G	270	GLN
1	G	286	TYR
1	H	178	LYS
1	H	212	GLU
1	H	267	LYS
1	H	283	TYR
1	I	74	ASN
1	I	81	HIS
1	I	178	LYS
1	I	209	LYS
1	I	233	ARG
1	I	250	VAL
1	I	281	ARG
1	K	11	LYS
1	K	209	LYS
1	K	213	ARG
1	K	234	GLU
1	K	236	LEU
1	K	276	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	184	GLN
1	A	255	ASN
1	B	74	ASN
1	C	17	GLN
1	C	261	HIS
1	D	141	GLN

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Mol	Chain	Res	Type
1	D	255	ASN
1	E	101	ASN
1	E	151	GLN
1	F	276	ASN
1	G	58	HIS
1	G	81	HIS
1	G	200	GLN
1	G	245	GLN
1	G	275	HIS
1	H	81	HIS
1	H	200	GLN
1	I	74	ASN
1	K	245	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](#)

10 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	26T	A	301	-	10,12,12	5.40	3 (30%)	9,17,17	2.29	6 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	26T	B	301	-	10,12,12	5.39	3 (30%)	9,17,17	2.31	6 (66%)
2	26T	C	301	-	10,12,12	5.27	3 (30%)	9,17,17	2.36	7 (77%)
2	26T	D	301	-	10,12,12	5.66	2 (20%)	9,17,17	2.37	6 (66%)
2	26T	E	301	-	10,12,12	5.35	3 (30%)	9,17,17	2.36	7 (77%)
2	26T	F	301	-	10,12,12	5.65	3 (30%)	9,17,17	2.42	7 (77%)
2	26T	G	301	-	10,12,12	5.22	3 (30%)	9,17,17	2.30	6 (66%)
2	26T	H	301	-	10,12,12	5.49	3 (30%)	9,17,17	2.34	6 (66%)
2	26T	I	301	-	10,12,12	5.52	3 (30%)	9,17,17	2.30	6 (66%)
2	26T	K	301	-	10,12,12	5.49	3 (30%)	9,17,17	2.31	6 (66%)

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	26T	A	301	-	-	0/13/14/14	0/0/0/0
2	26T	B	301	-	-	0/13/14/14	0/0/0/0
2	26T	C	301	-	-	0/13/14/14	0/0/0/0
2	26T	D	301	-	-	0/13/14/14	0/0/0/0
2	26T	E	301	-	-	0/13/14/14	0/0/0/0
2	26T	F	301	-	-	0/13/14/14	0/0/0/0
2	26T	G	301	-	-	0/13/14/14	0/0/0/0
2	26T	H	301	-	-	0/13/14/14	0/0/0/0
2	26T	I	301	-	-	0/13/14/14	0/0/0/0
2	26T	K	301	-	-	0/13/14/14	0/0/0/0

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	26T	O06-C05	-15.99	1.32	1.43
2	D	301	26T	O06-C05	-15.76	1.32	1.43
2	I	301	26T	O06-C05	-14.99	1.32	1.43
2	K	301	26T	O06-C05	-14.90	1.33	1.43
2	H	301	26T	O06-C05	-14.66	1.33	1.43
2	B	301	26T	O06-C05	-14.44	1.33	1.43
2	A	301	26T	O06-C05	-14.26	1.33	1.43
2	E	301	26T	O06-C05	-14.09	1.33	1.43
2	C	301	26T	O06-C05	-14.01	1.33	1.43
2	G	301	26T	O06-C05	-13.23	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	26T	C05-C04	2.40	1.55	1.51
2	B	301	26T	C05-C04	2.82	1.56	1.51
2	K	301	26T	C05-C04	2.98	1.56	1.51
2	I	301	26T	C05-C04	3.22	1.57	1.51
2	H	301	26T	C05-C04	3.31	1.57	1.51
2	A	301	26T	C05-C04	3.41	1.57	1.51
2	E	301	26T	C05-C04	3.76	1.57	1.51
2	C	301	26T	C05-C04	3.78	1.57	1.51
2	G	301	26T	C05-C04	3.86	1.58	1.51
2	F	301	26T	P07-O06	7.35	1.84	1.60
2	C	301	26T	P07-O06	7.88	1.86	1.60
2	D	301	26T	P07-O06	8.04	1.87	1.60
2	I	301	26T	P07-O06	8.11	1.87	1.60
2	K	301	26T	P07-O06	8.13	1.87	1.60
2	E	301	26T	P07-O06	8.30	1.88	1.60
2	B	301	26T	P07-O06	8.34	1.88	1.60
2	A	301	26T	P07-O06	8.45	1.88	1.60
2	H	301	26T	P07-O06	8.46	1.88	1.60
2	G	301	26T	P07-O06	8.82	1.89	1.60

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	301	26T	O06-P07-O10	-3.09	99.28	107.14
2	D	301	26T	O06-P07-O10	-2.99	99.53	107.14
2	D	301	26T	O13-C02-C01	-2.86	115.41	121.01
2	F	301	26T	O13-C02-C01	-2.86	115.42	121.01
2	I	301	26T	O06-P07-O10	-2.83	99.93	107.14
2	F	301	26T	O06-P07-O10	-2.82	99.96	107.14
2	C	301	26T	O13-C02-C01	-2.80	115.54	121.01
2	G	301	26T	O13-C02-C01	-2.79	115.56	121.01
2	H	301	26T	O13-C02-C01	-2.76	115.61	121.01
2	G	301	26T	O06-P07-O10	-2.75	100.14	107.14
2	B	301	26T	O13-C02-C01	-2.75	115.63	121.01
2	F	301	26T	O08-P07-O06	-2.68	98.85	106.56
2	K	301	26T	O13-C02-C01	-2.66	115.80	121.01
2	I	301	26T	O13-C02-C01	-2.66	115.80	121.01
2	A	301	26T	O06-P07-O10	-2.66	100.37	107.14
2	A	301	26T	O13-C02-C01	-2.65	115.82	121.01
2	K	301	26T	O08-P07-O06	-2.58	99.12	106.56
2	B	301	26T	O08-P07-O06	-2.57	99.16	106.56
2	E	301	26T	O13-C02-C01	-2.55	116.03	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	26T	O09-P07-O06	-2.54	99.25	106.56
2	I	301	26T	O08-P07-O06	-2.49	99.38	106.56
2	A	301	26T	O08-P07-O06	-2.43	99.57	106.56
2	E	301	26T	O08-P07-O06	-2.42	99.60	106.56
2	E	301	26T	O06-P07-O10	-2.36	101.14	107.14
2	C	301	26T	O08-P07-O06	-2.35	99.80	106.56
2	G	301	26T	O08-P07-O06	-2.31	99.90	106.56
2	H	301	26T	O08-P07-O06	-2.18	100.29	106.56
2	D	301	26T	O08-P07-O06	-2.13	100.44	106.56
2	K	301	26T	O09-P07-O06	-2.04	100.69	106.56
2	A	301	26T	C05-C04-C03	2.01	122.04	118.22
2	B	301	26T	O09-P07-O10	2.03	117.10	110.58
2	I	301	26T	O09-P07-O10	2.03	117.13	110.58
2	C	301	26T	O09-P07-O10	2.05	117.18	110.58
2	F	301	26T	O09-P07-O10	2.08	117.28	110.58
2	E	301	26T	O09-P07-O10	2.09	117.30	110.58
2	K	301	26T	O09-P07-O10	2.11	117.36	110.58
2	B	301	26T	O08-P07-O09	2.11	115.42	107.38
2	F	301	26T	C05-C04-C03	2.12	122.24	118.22
2	H	301	26T	C05-C04-C03	2.12	122.24	118.22
2	E	301	26T	O08-P07-O10	2.12	117.40	110.58
2	K	301	26T	O08-P07-O09	2.13	115.49	107.38
2	C	301	26T	C05-C04-C03	2.21	122.41	118.22
2	G	301	26T	C05-C04-C03	2.24	122.47	118.22
2	C	301	26T	O08-P07-O09	2.24	115.92	107.38
2	D	301	26T	C05-C04-C03	2.28	122.55	118.22
2	A	301	26T	O08-P07-O09	2.31	116.16	107.38
2	B	301	26T	C05-C04-C03	2.38	122.74	118.22
2	I	301	26T	O08-P07-O09	2.42	116.58	107.38
2	H	301	26T	O08-P07-O09	2.51	116.93	107.38
2	G	301	26T	O08-P07-O09	2.51	116.95	107.38
2	F	301	26T	O08-P07-O09	2.55	117.10	107.38
2	D	301	26T	O08-P07-O09	2.56	117.12	107.38
2	E	301	26T	C05-C04-C03	2.63	123.22	118.22
2	I	301	26T	C01-C02-C03	2.99	121.89	118.03
2	F	301	26T	C01-C02-C03	3.00	121.90	118.03
2	D	301	26T	C01-C02-C03	3.04	121.95	118.03
2	B	301	26T	C01-C02-C03	3.05	121.97	118.03
2	E	301	26T	C01-C02-C03	3.08	122.00	118.03
2	H	301	26T	C01-C02-C03	3.14	122.07	118.03
2	K	301	26T	C01-C02-C03	3.19	122.14	118.03
2	A	301	26T	C01-C02-C03	3.20	122.15	118.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	301	26T	C01-C02-C03	3.26	122.23	118.03
2	C	301	26T	C01-C02-C03	3.26	122.24	118.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	26T	1	0
2	B	301	26T	2	0
2	D	301	26T	4	0
2	E	301	26T	2	0
2	F	301	26T	1	0
2	G	301	26T	2	0
2	H	301	26T	3	0
2	I	301	26T	3	0
2	K	301	26T	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	281/293 (95%)	0.94	37 (13%) 4 4	31, 50, 104, 156	0
1	B	281/293 (95%)	0.31	7 (2%) 61 65	19, 35, 56, 79	0
1	C	281/293 (95%)	0.78	30 (10%) 8 8	31, 49, 85, 145	0
1	D	281/293 (95%)	1.26	54 (19%) 2 1	37, 61, 113, 137	0
1	E	281/293 (95%)	0.48	16 (5%) 27 31	18, 37, 71, 124	0
1	F	280/293 (95%)	0.25	6 (2%) 67 71	19, 33, 53, 99	0
1	G	281/293 (95%)	1.17	53 (18%) 2 1	33, 58, 109, 201	0
1	H	281/293 (95%)	0.88	41 (14%) 3 3	30, 51, 90, 107	0
1	I	281/293 (95%)	0.44	18 (6%) 23 25	20, 37, 77, 147	0
1	K	281/293 (95%)	0.80	27 (9%) 10 11	28, 49, 88, 119	0
All	All	2809/2930 (95%)	0.73	289 (10%) 9 9	18, 45, 92, 201	0

All (289) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	10	GLY	12.0
1	G	287	LEU	9.6
1	H	283	TYR	8.4
1	E	181	VAL	8.3
1	D	287	LEU	7.9
1	C	289	GLU	7.8
1	I	10	GLY	7.6
1	C	288	SER	7.1
1	G	288	SER	7.0
1	A	206	TYR	6.8
1	D	259	SER	6.7
1	C	177	GLY	6.4
1	A	208	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
1	I	9	ASP	6.2
1	A	286	TYR	6.0
1	D	252	MET	5.9
1	C	286	TYR	5.8
1	C	285	LEU	5.7
1	A	13	PHE	5.7
1	D	179	ASP	5.7
1	C	287	LEU	5.6
1	D	178	LYS	5.5
1	H	176	VAL	5.4
1	G	186	TYR	5.3
1	D	10	GLY	5.3
1	D	181	VAL	5.2
1	H	233	ARG	5.1
1	A	205	TYR	5.1
1	D	66	THR	5.1
1	A	283	TYR	5.1
1	D	9	ASP	5.1
1	G	19	GLN	5.0
1	D	283	TYR	4.9
1	I	288	SER	4.8
1	G	16	ASP	4.7
1	G	252	MET	4.7
1	H	9	ASP	4.7
1	G	181	VAL	4.7
1	D	233	ARG	4.7
1	D	265	MET	4.6
1	K	254	ARG	4.6
1	A	179	ASP	4.6
1	K	283	TYR	4.5
1	D	263	VAL	4.5
1	E	180	MET	4.4
1	C	181	VAL	4.4
1	K	176	VAL	4.4
1	A	274	HIS	4.4
1	I	276	ASN	4.4
1	G	178	LYS	4.3
1	K	75	ILE	4.3
1	A	211	PHE	4.3
1	K	177	GLY	4.3
1	G	283	TYR	4.3
1	K	178	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	285	LEU	4.2
1	D	274	HIS	4.2
1	A	10	GLY	4.2
1	G	207	VAL	4.1
1	E	65	THR	4.1
1	D	246	GLY	4.1
1	E	182	ARG	4.0
1	A	184	GLN	4.0
1	G	273	VAL	3.9
1	D	279	ALA	3.9
1	H	178	LYS	3.9
1	A	273	VAL	3.9
1	I	178	LYS	3.8
1	G	276	ASN	3.8
1	A	289	GLU	3.8
1	K	255	ASN	3.8
1	A	285	LEU	3.8
1	E	116	ALA	3.8
1	G	64	PRO	3.8
1	H	206	TYR	3.8
1	G	264	ALA	3.8
1	D	176	VAL	3.7
1	H	279	ALA	3.7
1	G	268	ALA	3.7
1	D	288	SER	3.7
1	D	251	ASP	3.7
1	K	9	ASP	3.6
1	G	180	MET	3.6
1	E	10	GLY	3.6
1	H	289	GLU	3.6
1	K	116	ALA	3.6
1	G	286	TYR	3.6
1	D	205	TYR	3.6
1	C	66	THR	3.5
1	C	9	ASP	3.5
1	H	47	LYS	3.5
1	A	275	HIS	3.4
1	D	67	GLY	3.4
1	I	180	MET	3.4
1	K	289	GLU	3.4
1	C	77	PRO	3.4
1	D	200	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	H	282	ALA	3.4
1	C	258	GLN	3.3
1	G	189	LEU	3.3
1	H	179	ASP	3.4
1	G	245	GLN	3.3
1	D	272	VAL	3.3
1	D	177	GLY	3.3
1	G	49	GLY	3.3
1	G	275	HIS	3.3
1	D	180	MET	3.3
1	D	229	LYS	3.3
1	H	175	GLY	3.2
1	K	261	HIS	3.2
1	D	250	VAL	3.2
1	A	213	ARG	3.2
1	H	236	LEU	3.2
1	C	179	ASP	3.1
1	D	277	GLU	3.1
1	H	184	GLN	3.1
1	A	176	VAL	3.1
1	G	44	PHE	3.1
1	H	285	LEU	3.1
1	G	102	ARG	3.1
1	H	281	ARG	3.1
1	A	282	ALA	3.1
1	H	225	ALA	3.1
1	H	224	ILE	3.1
1	K	114	ILE	3.1
1	F	180	MET	3.1
1	G	84	VAL	3.1
1	G	234	GLU	3.1
1	H	266	MET	3.0
1	H	24	PHE	3.0
1	I	176	VAL	3.0
1	D	275	HIS	3.0
1	B	10	GLY	3.0
1	C	178	LYS	3.0
1	G	282	ALA	3.0
1	D	19	GLN	3.0
1	H	18	PRO	3.0
1	C	71	ILE	3.0
1	D	235	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	13	PHE	3.0
1	G	289	GLU	3.0
1	H	268	ALA	3.0
1	G	261	HIS	3.0
1	D	231	PRO	2.9
1	D	262	PRO	2.9
1	D	276	ASN	2.9
1	D	286	TYR	2.9
1	C	180	MET	2.9
1	A	181	VAL	2.8
1	G	228	LYS	2.8
1	D	68	LEU	2.8
1	K	281	ARG	2.8
1	D	76	ALA	2.8
1	E	287	LEU	2.8
1	K	180	MET	2.8
1	D	254	ARG	2.8
1	G	78	LEU	2.8
1	E	286	TYR	2.8
1	K	252	MET	2.8
1	D	225	ALA	2.8
1	G	179	ASP	2.7
1	G	285	LEU	2.7
1	F	86	MET	2.7
1	H	13	PHE	2.7
1	K	179	ASP	2.7
1	D	270	GLN	2.7
1	C	278	THR	2.7
1	A	64	PRO	2.7
1	A	260	ASP	2.7
1	D	242	ALA	2.7
1	G	208	GLU	2.7
1	A	16	ASP	2.7
1	A	264	ALA	2.7
1	K	276	ASN	2.7
1	H	65	THR	2.6
1	A	281	ARG	2.6
1	A	266	MET	2.6
1	H	210	GLY	2.6
1	K	253	GLY	2.6
1	K	260	ASP	2.6
1	H	68	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	287	LEU	2.6
1	I	177	GLY	2.6
1	G	185	ARG	2.6
1	G	56	PHE	2.6
1	G	235	ALA	2.6
1	K	209	LYS	2.6
1	C	205	TYR	2.6
1	G	259	SER	2.5
1	C	260	ASP	2.5
1	F	11	LYS	2.5
1	G	202	ILE	2.5
1	C	131	VAL	2.5
1	G	269	VAL	2.5
1	G	18	PRO	2.5
1	E	144	ILE	2.5
1	H	205	TYR	2.5
1	A	268	ALA	2.5
1	A	207	VAL	2.5
1	G	257	PHE	2.5
1	G	260	ASP	2.5
1	K	12	ASP	2.5
1	H	10	GLY	2.5
1	I	281	ARG	2.5
1	D	258	GLN	2.4
1	D	278	THR	2.4
1	H	246	GLY	2.4
1	C	268	ALA	2.4
1	D	282	ALA	2.4
1	B	179	ASP	2.4
1	H	275	HIS	2.4
1	I	181	VAL	2.4
1	G	43	ILE	2.4
1	H	177	GLY	2.4
1	F	65	THR	2.4
1	G	89	ARG	2.4
1	A	272	VAL	2.4
1	H	182	ARG	2.4
1	A	210	GLY	2.4
1	K	285	LEU	2.4
1	K	233	ARG	2.4
1	C	242	ALA	2.4
1	D	255	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	286	TYR	2.4
1	I	286	TYR	2.4
1	E	275	HIS	2.4
1	E	289	GLU	2.4
1	A	261	HIS	2.3
1	G	284	GLU	2.3
1	D	127	MET	2.3
1	C	283	TYR	2.3
1	B	177	GLY	2.3
1	A	235	ALA	2.3
1	D	43	ILE	2.3
1	G	17	GLN	2.3
1	I	285	LEU	2.3
1	E	142	VAL	2.3
1	H	74	ASN	2.3
1	E	179	ASP	2.3
1	C	55	ALA	2.3
1	A	204	THR	2.3
1	C	75	ILE	2.3
1	D	234	GLU	2.3
1	A	276	ASN	2.3
1	D	81	HIS	2.3
1	I	287	LEU	2.3
1	C	280	ASP	2.2
1	I	210	GLY	2.2
1	A	186	TYR	2.2
1	E	211	PHE	2.2
1	G	79	PHE	2.2
1	H	284	GLU	2.2
1	I	175	GLY	2.2
1	G	263	VAL	2.2
1	B	119	SER	2.2
1	I	11	LYS	2.2
1	K	61	PHE	2.2
1	C	26	LEU	2.2
1	H	145	GLY	2.2
1	H	14	ARG	2.2
1	C	95	VAL	2.2
1	G	251	ASP	2.2
1	B	288	SER	2.1
1	B	180	MET	2.1
1	I	224	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	87	CYS	2.1
1	D	174	THR	2.1
1	C	279	ALA	2.1
1	B	281	ARG	2.1
1	G	172	ALA	2.1
1	D	266	MET	2.1
1	H	83	ASP	2.1
1	H	17	GLN	2.1
1	C	189	LEU	2.1
1	H	15	THR	2.1
1	K	288	SER	2.1
1	K	11	LYS	2.1
1	D	57	ASP	2.1
1	A	203	ALA	2.1
1	A	19	GLN	2.1
1	G	267	LYS	2.1
1	C	263	VAL	2.0
1	D	107	ARG	2.0
1	A	280	ASP	2.0
1	H	45	ASN	2.0
1	G	81	HIS	2.0
1	K	256	ILE	2.0
1	E	115	LEU	2.0
1	I	74	ASN	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( $\text{\AA}^2$ )	Q<0.9
2	26T	B	301	13/13	0.92	0.22	1.04	39,46,55,56	0
2	26T	E	301	13/13	0.88	0.20	0.68	43,49,72,72	0
2	26T	F	301	13/13	0.87	0.18	0.31	37,63,67,69	0
2	26T	C	301	13/13	0.90	0.20	0.27	31,40,93,93	0
2	26T	A	301	13/13	0.84	0.22	0.15	50,55,86,86	0
2	26T	H	301	13/13	0.90	0.22	0.04	53,58,67,68	0
2	26T	I	301	13/13	0.90	0.17	-0.04	40,55,69,69	0
2	26T	K	301	13/13	0.80	0.23	-0.09	47,58,72,73	0
2	26T	G	301	13/13	0.80	0.19	-0.68	45,60,90,91	0
2	26T	D	301	13/13	0.82	0.18	-0.94	49,66,69,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.