Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2016 – 01:15 PM EST

PDB ID	:	5D39
Title	:	Transcription factor-DNA complex
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Deposited on	:	2015-08-06
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

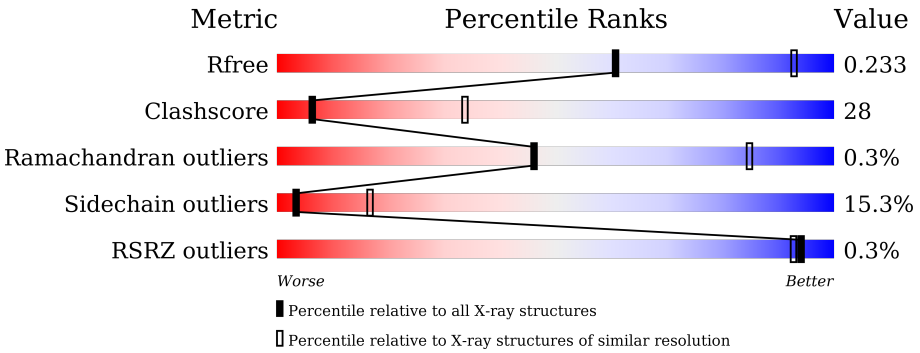
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	539	51% 33% 6% 9%
1	B	539	52% 32% 6% 10%
1	C	539	52% 30% 8% 10%
1	D	539	% 52% 29% 9% 10%
2	F	21	62% 29% 10%
2	N	21	62% 29% 10%

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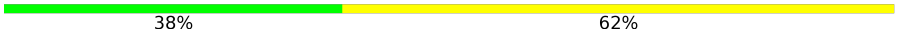
Mol	Chain	Length	Quality of chain
3	E	21	
3	M	21	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17397 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 Signal transducer and activator of transcription 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	P	S	0	0	0
			3891	2478	683	713	1	16			
1	B	484	Total	C	N	O	P	S	0	0	0
			3850	2451	674	708	1	16			
1	C	484	Total	C	N	O	P	S	0	0	0
			3851	2454	673	707	1	16			
1	D	487	Total	C	N	O	P	S	0	0	0
			3877	2468	678	714	1	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	SER	-	expression tag	UNP P42226
A	121	ASN	-	expression tag	UNP P42226
A	122	ALA	-	expression tag	UNP P42226
B	120	SER	-	expression tag	UNP P42226
B	121	ASN	-	expression tag	UNP P42226
B	122	ALA	-	expression tag	UNP P42226
C	120	SER	-	expression tag	UNP P42226
C	121	ASN	-	expression tag	UNP P42226
C	122	ALA	-	expression tag	UNP P42226
D	120	SER	-	expression tag	UNP P42226
D	121	ASN	-	expression tag	UNP P42226
D	122	ALA	-	expression tag	UNP P42226

- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*CP*TP*GP*TP*CP*TP*TP*CP*CP *AP*GP*GP*AP*AP*AP*TP*CP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	21	Total	C	N	O	P	0	0	0
			425	204	72	128	21			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	21	Total	C	N	O	P	0	0	0
			425	204	72	128	21			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*TP*GP*GP*AP*TP*TP*TP*CP*CP *TP*GP*GP*AP*AP*GP*AP*CP*AP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	21	Total	C	N	O	P	0	0	0
			436	207	84	124	21			
3	E	21	Total	C	N	O	P	0	0	0
			436	207	84	124	21			

- Molecule 4 is water.

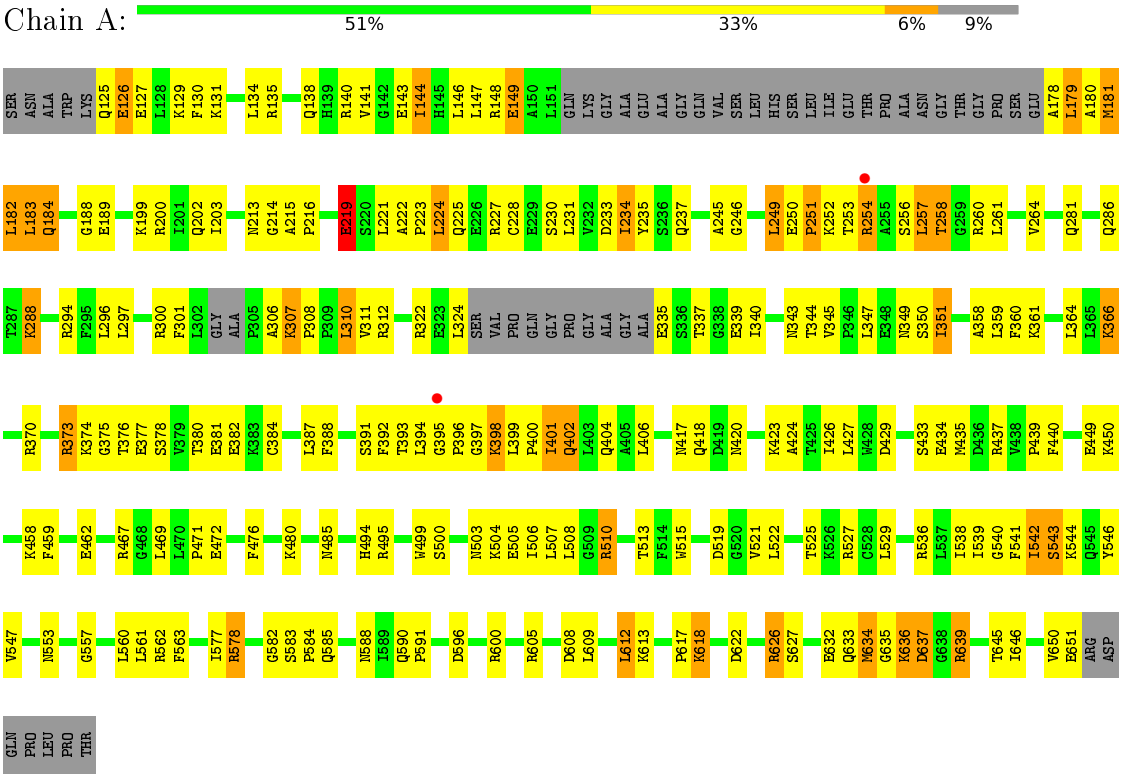
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	55	Total	O	0	0
			55	55		
4	C	50	Total	O	0	0
			50	50		
4	D	31	Total	O	0	0
			31	31		
4	N	4	Total	O	0	0
			4	4		
4	M	2	Total	O	0	0
			2	2		
4	E	1	Total	O	0	0
			1	1		
4	F	2	Total	O	0	0
			2	2		

3 Residue-property plots (i)

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.

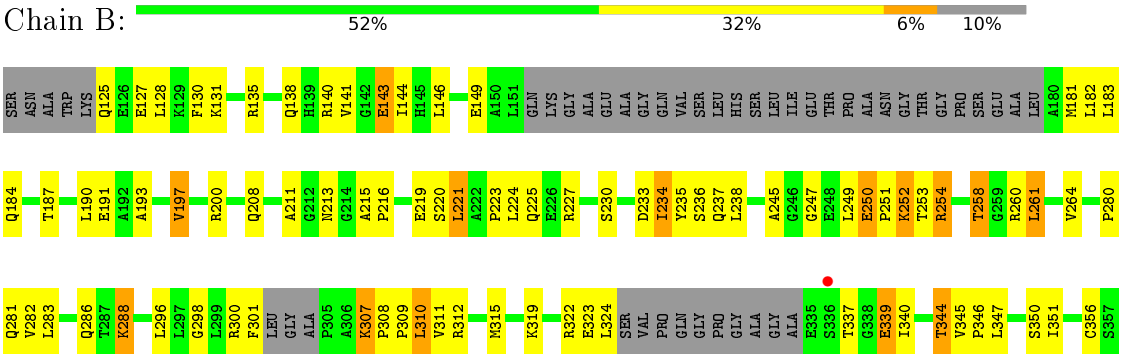
- Molecule 1: Signal transducer and activator of transcription 6

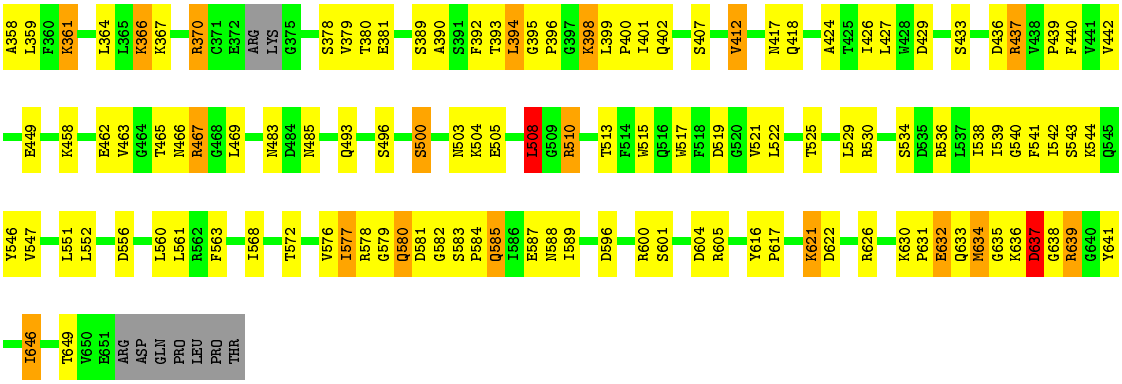
Chain A:



- Molecule 1: Signal transducer and activator of transcription 6

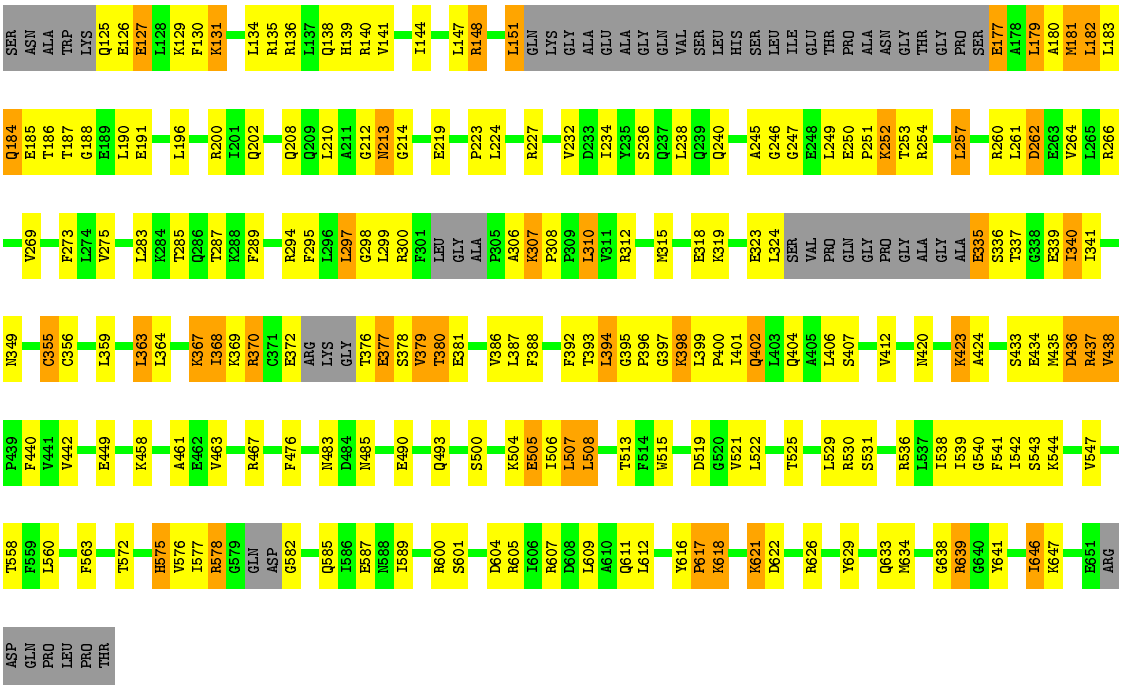
Chain B:





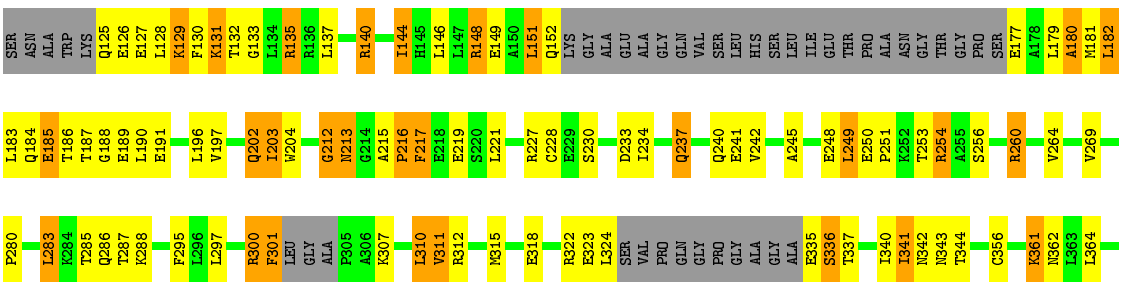
• Molecule 1: Signal transducer and activator of transcription 6

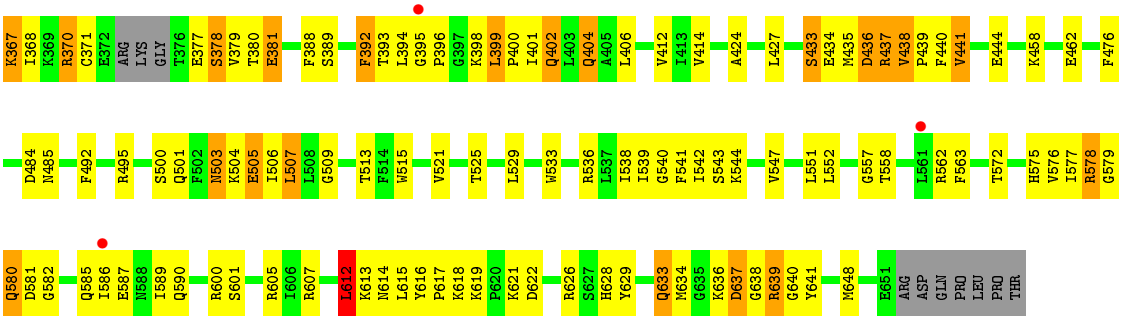
Chain C:



• Molecule 1: Signal transducer and activator of transcription 6

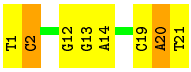
Chain D:





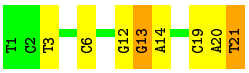
• Molecule 2: DNA (5'-D(P*TP*CP*TP*GP*TP*CP*TP*TP*CP*CP*AP*GP*GP*AP*AP*AP*TP*CP*CP*AP*T)-3')

Chain N:



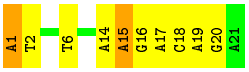
• Molecule 2: DNA (5'-D(P*TP*CP*TP*GP*TP*CP*TP*TP*CP*CP*AP*GP*GP*AP*AP*AP*TP*CP*CP*AP*T)-3')

Chain F:



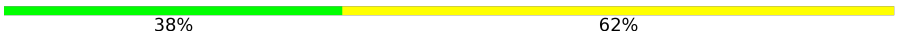
• Molecule 3: DNA (5'-D(P*AP*TP*GP*GP*AP*TP*TP*TP*CP*CP*TP*GP*GP*AP*AP*GP*AP*CP*AP*GP*A)-3')

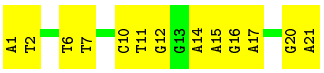
Chain M:



• Molecule 3: DNA (5'-D(P*AP*TP*GP*GP*AP*TP*TP*TP*CP*CP*TP*GP*GP*AP*AP*GP*AP*CP*AP*GP*A)-3')

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	68.39Å 94.70Å 145.64Å 79.62° 78.31° 89.58°	Depositor
Resolution (Å)	44.12 – 3.20 44.12 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.12-3.20) 89.4 (44.12-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.210 , 0.236 0.228 , 0.233	Depositor DCC
R_{free} test set	2622 reflections (4.84%)	DCC
Wilson B-factor (Å^2)	92.8	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.095 for h,-k,h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	17397	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: PTR

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	0.33	1/3944 (0.0%)	0.61	0/5316
1	B	0.33	1/3902 (0.0%)	0.61	2/5259 (0.0%)
1	C	0.33	0/3902	0.63	3/5258 (0.1%)
1	D	0.32	0/3929	0.62	3/5296 (0.1%)
2	F	0.80	0/474	1.18	2/728 (0.3%)
2	N	0.97	2/474 (0.4%)	1.28	4/728 (0.5%)
3	E	0.68	0/490	1.05	0/755
3	M	0.71	0/490	1.18	3/755 (0.4%)
All	All	0.41	4/17605 (0.0%)	0.71	17/24095 (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	A	0	1
1	B	0	1
1	D	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	1	DT	C1'-N1	6.80	1.58	1.49
2	N	1	DT	C2-O2	-6.56	1.17	1.22
1	B	216	PRO	N-CD	5.22	1.55	1.47
1	A	251	PRO	N-CD	5.11	1.55	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	20	DA	O4'-C1'-N9	11.72	116.20	108.00
1	B	508	LEU	CA-CB-CG	9.04	136.10	115.30
3	M	1	DA	O4'-C1'-N9	8.43	113.90	108.00
1	C	151	LEU	CA-CB-CG	7.03	131.46	115.30
2	N	20	DA	C1'-O4'-C4'	-6.41	103.69	110.10
1	C	182	LEU	CA-CB-CG	6.29	129.76	115.30
3	M	2	DT	O4'-C1'-N1	6.06	112.24	108.00
2	F	13	DG	P-O3'-C3'	5.84	126.70	119.70
2	N	2	DC	O4'-C1'-N1	5.81	112.06	108.00
1	D	612	LEU	CA-CB-CG	5.75	128.53	115.30
1	C	182	LEU	CB-CG-CD2	5.73	120.74	111.00
1	B	215	ALA	C-N-CD	5.68	140.33	128.40
2	N	1	DT	O4'-C1'-N1	5.63	111.94	108.00
2	F	21	DT	N3-C4-O4	5.19	123.01	119.90
3	M	15	DA	O4'-C1'-N9	5.19	111.63	108.00
1	D	507	LEU	CA-CB-CG	5.12	127.08	115.30
1	D	212	GLY	N-CA-C	-5.02	100.55	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	219	GLU	Peptide
1	B	245	ALA	Peptide
1	D	180	ALA	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	3891	0	3973	241	0
1	B	3850	0	3918	182	0
1	C	3851	0	3925	246	0
1	D	3877	0	3946	241	0
2	F	425	0	239	16	0
2	N	425	0	239	13	0
3	E	436	0	237	12	0
3	M	436	0	237	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	61	0	0	47	0
4	B	55	0	0	36	0
4	C	50	0	0	78	0
4	D	31	0	0	32	0
4	E	1	0	0	1	0
4	F	2	0	0	4	0
4	M	2	0	0	3	0
4	N	4	0	0	0	0
All	All	17397	0	16714	943	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (943) 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:179:LEU:HD23	1:D:182:LEU:CB	1.44	1.46
1:D:179:LEU:CD2	1:D:182:LEU:HD22	1.46	1.43
1:D:179:LEU:HD21	1:D:182:LEU:CD2	1.50	1.40
1:A:246:GLY:HA2	1:A:249:LEU:CD1	1.50	1.39
1:A:245:ALA:O	1:A:249:LEU:CD2	1.69	1.39
1:D:437:ARG:HH21	1:D:440:PHE:CA	1.36	1.38
1:A:246:GLY:O	1:A:249:LEU:CG	1.71	1.35
1:D:367:LYS:CE	1:D:367:LYS:HA	1.49	1.35
1:A:246:GLY:CA	1:A:249:LEU:HD11	1.56	1.35
1:A:250:GLU:CD	1:A:251:PRO:HD2	1.47	1.33
1:D:367:LYS:CA	1:D:367:LYS:HE2	1.49	1.33
1:A:397:GLY:HA3	4:A:741:HOH:O	1.19	1.32
1:B:572:THR:HA	4:B:721:HOH:O	1.29	1.32
1:A:125:GLN:HG3	4:A:750:HOH:O	1.24	1.28
1:A:250:GLU:OE2	1:A:251:PRO:CD	1.80	1.28
1:C:437:ARG:HA	4:C:735:HOH:O	1.28	1.26
1:B:213:ASN:ND2	1:B:427:LEU:HD12	1.48	1.26
1:C:542:ILE:HD13	1:C:547:VAL:CG1	1.64	1.25
1:C:647:LYS:HG3	4:C:736:HOH:O	1.35	1.24
1:C:273:PHE:HA	4:C:717:HOH:O	1.37	1.23
1:D:437:ARG:HD2	1:D:441:VAL:O	1.38	1.21
1:D:492:PHE:HA	4:D:711:HOH:O	1.38	1.20
1:C:262:ASP:HB3	4:C:711:HOH:O	1.41	1.19
1:D:179:LEU:CD2	1:D:182:LEU:CB	2.20	1.19
1:A:306:ALA:HB3	4:A:729:HOH:O	1.43	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ARG:HB2	4:A:733:HOH:O	1.41	1.17
1:A:245:ALA:O	1:A:249:LEU:HD21	1.31	1.17
1:A:250:GLU:OE1	1:A:251:PRO:HD2	1.42	1.16
1:C:179:LEU:HD11	4:C:746:HOH:O	1.43	1.16
1:B:200:ARG:HD2	4:B:742:HOH:O	1.47	1.15
1:C:407:SER:HA	4:C:722:HOH:O	1.47	1.15
3:M:17:DA:H2"	4:M:102:HOH:O	1.48	1.13
1:C:359:LEU:HB3	4:C:706:HOH:O	1.48	1.11
1:D:437:ARG:HH21	1:D:440:PHE:HA	1.09	1.11
1:D:179:LEU:CD2	1:D:182:LEU:CD2	2.15	1.11
1:D:180:ALA:HA	1:D:183:LEU:HB2	1.33	1.10
1:B:582:GLY:HA3	4:B:736:HOH:O	1.53	1.09
1:D:437:ARG:NH2	1:D:440:PHE:HA	1.68	1.09
1:A:250:GLU:CD	1:A:251:PRO:CD	2.18	1.09
1:B:587:GLU:OE2	1:D:636:LYS:NZ	1.85	1.09
1:C:542:ILE:CD1	1:C:547:VAL:HG12	1.81	1.08
1:D:437:ARG:CD	1:D:441:VAL:O	2.01	1.07
1:D:435:MET:HG2	4:D:730:HOH:O	1.53	1.06
1:C:379:VAL:HG12	4:C:732:HOH:O	1.53	1.06
1:A:553:ASN:HB2	4:A:719:HOH:O	1.52	1.06
1:A:577:ILE:HG13	1:A:578:ARG:HB3	1.34	1.05
1:B:213:ASN:ND2	1:B:427:LEU:CD1	2.20	1.05
1:D:437:ARG:NH2	1:D:440:PHE:CA	2.17	1.05
1:A:245:ALA:O	1:A:249:LEU:HD22	1.55	1.05
1:B:213:ASN:HD21	1:B:427:LEU:HD12	1.01	1.05
1:A:249:LEU:HD23	1:A:249:LEU:H	1.18	1.04
1:A:542:ILE:HG12	1:A:547:VAL:HG12	1.40	1.04
1:B:366:LYS:HD2	1:B:366:LYS:C	1.77	1.04
1:A:250:GLU:OE2	1:A:251:PRO:CG	2.05	1.03
1:A:632:GLU:OE2	1:A:632:GLU:N	1.91	1.03
1:A:562:ARG:HD3	4:A:724:HOH:O	1.57	1.03
1:D:151:LEU:HD11	4:D:702:HOH:O	1.55	1.03
1:C:483:ASN:OD1	1:C:508:LEU:HD11	1.59	1.02
1:B:632:GLU:OE2	1:B:632:GLU:N	1.93	1.02
1:A:246:GLY:CA	1:A:249:LEU:HD21	1.90	1.02
1:A:246:GLY:O	1:A:249:LEU:HG	0.85	1.02
1:A:507:LEU:HB2	1:A:510:ARG:HB2	1.38	1.01
1:A:250:GLU:OE2	1:A:251:PRO:N	1.92	1.01
1:C:507:LEU:HD12	1:C:507:LEU:H	1.26	1.00
1:C:318:GLU:HB3	4:C:710:HOH:O	1.61	0.99
1:A:249:LEU:HD12	1:A:254:ARG:HG3	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LEU:HD23	1:D:182:LEU:HB2	1.01	0.98
1:D:379:VAL:HG23	3:E:6:DT:OP1	1.63	0.98
1:D:179:LEU:CD2	1:D:182:LEU:CG	2.41	0.98
1:A:245:ALA:C	1:A:249:LEU:HD21	1.85	0.97
1:B:366:LYS:CD	1:B:366:LYS:C	2.32	0.97
1:C:177:GLU:HB3	4:C:734:HOH:O	1.63	0.96
1:D:315:MET:HG2	1:D:340:ILE:HD11	1.47	0.96
1:A:246:GLY:C	1:A:249:LEU:HD21	1.86	0.96
1:B:223:PRO:HD2	4:B:725:HOH:O	1.63	0.96
1:D:633:GLN:OE1	1:D:634:MET:N	1.97	0.95
1:D:179:LEU:HD23	1:D:182:LEU:CG	1.96	0.95
1:D:437:ARG:HH21	1:D:440:PHE:C	1.68	0.95
1:A:310:LEU:HD22	1:A:311:VAL:N	1.82	0.95
1:A:188:GLY:HA2	4:A:737:HOH:O	1.66	0.95
1:A:246:GLY:C	1:A:249:LEU:CG	2.35	0.94
1:D:628:HIS:HD2	4:D:723:HOH:O	1.50	0.94
1:A:246:GLY:C	1:A:249:LEU:HG	1.86	0.94
1:D:324:LEU:HB3	4:D:728:HOH:O	1.68	0.93
1:D:179:LEU:CD2	1:D:182:LEU:HB3	1.98	0.93
1:A:246:GLY:C	1:A:249:LEU:CD2	2.37	0.93
1:A:189:GLU:HA	4:A:718:HOH:O	1.69	0.92
1:D:437:ARG:HE	1:D:441:VAL:N	1.66	0.92
1:D:125:GLN:HG3	4:D:726:HOH:O	1.69	0.92
1:D:542:ILE:HD13	1:D:547:VAL:HG13	1.51	0.91
1:A:311:VAL:HG12	1:A:345:VAL:O	1.70	0.91
1:C:381:GLU:OE2	1:C:504:LYS:NZ	2.03	0.90
1:A:250:GLU:OE2	1:A:251:PRO:HG2	1.69	0.90
2:N:2:DC:H42	3:M:20:DG:H1	1.20	0.90
1:C:140:ARG:HG2	1:C:186:THR:HG21	1.54	0.89
1:C:381:GLU:CD	1:C:504:LYS:NZ	2.26	0.89
1:D:617:PRO:HA	4:D:707:HOH:O	1.72	0.88
1:D:381:GLU:OE2	1:D:504:LYS:NZ	2.06	0.88
1:D:437:ARG:NE	1:D:441:VAL:O	2.07	0.87
1:C:224:LEU:CD1	4:C:727:HOH:O	2.23	0.87
1:B:366:LYS:HD2	1:B:366:LYS:O	1.73	0.86
1:A:543:SER:HA	4:A:709:HOH:O	1.74	0.86
1:B:442:VAL:HA	4:B:730:HOH:O	1.75	0.85
1:C:247:GLY:N	1:C:249:LEU:HD13	1.91	0.85
4:A:735:HOH:O	1:B:626:ARG:HB2	1.76	0.85
1:C:540:GLY:O	1:C:563:PHE:HD2	1.57	0.85
1:A:249:LEU:HB3	1:A:254:ARG:NH2	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:LYS:HB3	1:D:639:ARG:NH1	1.90	0.85
1:A:510:ARG:HD2	1:A:510:ARG:N	1.92	0.84
1:D:506:ILE:HG22	4:D:706:HOH:O	1.77	0.84
1:C:177:GLU:CB	4:C:734:HOH:O	2.18	0.84
1:C:275:VAL:HG21	4:C:722:HOH:O	1.77	0.84
1:B:310:LEU:HA	1:B:346:PRO:HA	1.57	0.84
1:C:582:GLY:CA	4:C:744:HOH:O	2.25	0.84
1:C:381:GLU:CD	1:C:504:LYS:HZ1	1.80	0.83
1:A:485:ASN:HA	4:A:748:HOH:O	1.78	0.83
1:A:249:LEU:HB2	1:A:254:ARG:CG	2.08	0.83
1:C:542:ILE:HD13	1:C:547:VAL:HG12	0.87	0.83
1:C:148:ARG:HE	1:C:245:ALA:HB2	1.43	0.83
1:C:493:GLN:HG3	4:C:713:HOH:O	1.79	0.82
1:C:582:GLY:HA3	4:C:744:HOH:O	1.77	0.82
1:C:585:GLN:O	4:C:701:HOH:O	1.95	0.82
1:A:249:LEU:HB3	1:A:254:ARG:CZ	2.09	0.82
1:B:319:LYS:O	4:B:701:HOH:O	1.96	0.82
1:B:633:GLN:O	1:B:634:MET:HG3	1.80	0.82
1:C:540:GLY:O	1:C:563:PHE:CD2	2.31	0.82
1:D:542:ILE:CD1	1:D:547:VAL:HG13	2.10	0.82
1:C:500:SER:HA	1:C:504:LYS:HB2	1.61	0.81
1:D:638:GLY:HA3	4:D:725:HOH:O	1.80	0.81
1:B:350:SER:HB2	4:B:740:HOH:O	1.81	0.81
1:C:359:LEU:CB	4:C:706:HOH:O	2.14	0.80
1:D:636:LYS:HB3	1:D:639:ARG:HH12	1.46	0.80
1:D:542:ILE:CD1	1:D:547:VAL:CG1	2.60	0.80
1:C:633:GLN:HA	1:C:634:MET:HB3	1.63	0.79
1:C:440:PHE:HE1	4:C:739:HOH:O	1.65	0.79
1:B:634:MET:SD	1:B:635:GLY:N	2.54	0.79
1:B:556:ASP:HB2	1:B:578:ARG:HG2	1.64	0.79
1:C:307:LYS:HD3	1:C:308:PRO:HD2	1.63	0.79
1:A:249:LEU:HB2	1:A:254:ARG:CD	2.13	0.78
1:C:376:THR:CG2	4:C:724:HOH:O	2.30	0.78
1:D:476:PHE:CD2	1:D:541:PHE:HB3	2.18	0.78
1:B:429:ASP:O	1:B:433:SER:OG	2.00	0.78
1:D:179:LEU:CD2	1:D:182:LEU:HB2	1.96	0.78
1:A:246:GLY:CA	1:A:249:LEU:CD2	2.61	0.78
1:C:376:THR:HG23	4:C:724:HOH:O	1.83	0.78
1:A:467:ARG:HD2	4:A:746:HOH:O	1.84	0.78
1:B:125:GLN:HG3	4:B:751:HOH:O	1.81	0.78
1:C:180:ALA:HB3	1:C:250:GLU:OE1	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:ILE:HD13	1:C:611:GLN:HB2	1.65	0.78
1:B:587:GLU:CD	1:D:636:LYS:NZ	2.36	0.77
1:C:249:LEU:HB3	4:C:726:HOH:O	1.84	0.77
1:B:637:ASP:O	1:B:641:PTR:O	2.02	0.77
1:C:539:ILE:HD12	1:C:560:LEU:HD13	1.65	0.77
1:A:578:ARG:NE	1:A:582:GLY:HA3	1.99	0.77
1:C:434:GLU:HB3	1:C:437:ARG:HB3	1.66	0.77
1:D:433:SER:OG	1:D:437:ARG:NH1	2.18	0.77
1:C:273:PHE:HD1	4:C:717:HOH:O	1.68	0.77
1:B:381:GLU:OE2	1:B:504:LYS:NZ	2.16	0.77
2:N:21:DT:O4	3:M:1:DA:N6	2.18	0.77
1:C:250:GLU:HG2	1:C:253:THR:CG2	2.16	0.76
1:C:394:LEU:CD2	4:C:738:HOH:O	2.32	0.76
1:B:485:ASN:HA	4:B:729:HOH:O	1.85	0.76
1:C:148:ARG:HE	1:C:245:ALA:CB	1.98	0.76
1:D:177:GLU:CA	4:D:702:HOH:O	2.34	0.76
1:D:542:ILE:HD13	1:D:547:VAL:CG1	2.15	0.76
1:A:214:GLY:HA2	4:A:744:HOH:O	1.84	0.76
1:B:366:LYS:CD	1:B:366:LYS:O	2.30	0.76
1:A:542:ILE:HG12	1:A:547:VAL:CG1	2.15	0.76
1:A:246:GLY:HA2	1:A:249:LEU:CG	2.16	0.75
1:D:242:VAL:HG13	1:D:254:ARG:HH11	1.50	0.75
1:A:500:SER:HA	1:A:504:LYS:HB2	1.68	0.75
1:C:190:LEU:HD23	1:C:234:ILE:HD11	1.68	0.75
1:C:507:LEU:HB2	1:C:508:LEU:CD2	2.17	0.75
1:C:508:LEU:HD22	1:C:508:LEU:N	2.02	0.75
1:C:177:GLU:HB2	4:C:726:HOH:O	1.86	0.75
1:B:359:LEU:O	1:B:361:LYS:NZ	2.19	0.75
1:A:310:LEU:O	1:A:345:VAL:O	2.04	0.75
1:A:577:ILE:HG13	1:A:578:ARG:CB	2.15	0.74
1:C:507:LEU:HD12	1:C:507:LEU:N	2.02	0.74
1:D:180:ALA:HA	1:D:183:LEU:H	1.51	0.74
1:C:476:PHE:CD2	1:C:541:PHE:HB3	2.23	0.74
1:C:381:GLU:OE1	1:C:504:LYS:NZ	2.19	0.74
1:A:538:ILE:HG22	1:A:540:GLY:N	2.03	0.74
1:C:249:LEU:HD23	4:C:726:HOH:O	1.87	0.74
1:B:125:GLN:CG	4:B:751:HOH:O	2.35	0.73
1:B:351:ILE:HG23	4:B:727:HOH:O	1.87	0.73
1:D:179:LEU:HD22	1:D:182:LEU:HB3	1.71	0.73
1:A:542:ILE:HG22	1:A:562:ARG:HB2	1.71	0.73
1:A:542:ILE:HG23	1:A:562:ARG:HE	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:ARG:HG2	4:B:746:HOH:O	1.88	0.72
1:D:577:ILE:O	1:D:585:GLN:N	2.21	0.72
1:A:324:LEU:HD12	4:A:727:HOH:O	1.89	0.72
1:C:190:LEU:HG	4:C:737:HOH:O	1.87	0.72
1:D:180:ALA:CA	1:D:183:LEU:H	2.02	0.72
1:D:437:ARG:NH2	1:D:440:PHE:CB	2.52	0.72
1:B:538:ILE:HG22	1:B:540:GLY:N	2.04	0.72
1:D:540:GLY:O	1:D:563:PHE:HD2	1.71	0.72
1:A:311:VAL:O	1:A:360:PHE:HZ	1.73	0.72
1:B:467:ARG:CG	4:B:746:HOH:O	2.38	0.72
3:M:18:DC:C6	4:M:102:HOH:O	2.44	0.71
1:A:246:GLY:CA	1:A:249:LEU:CG	2.68	0.71
1:D:180:ALA:HA	1:D:183:LEU:CB	2.15	0.71
1:D:639:ARG:CZ	1:D:640:GLY:H	2.04	0.71
1:A:542:ILE:CG2	1:A:562:ARG:HE	2.04	0.70
1:C:266:ARG:CD	4:C:747:HOH:O	2.39	0.70
1:D:310:LEU:CD1	4:D:704:HOH:O	2.38	0.70
1:B:127:GLU:HG2	1:B:227:ARG:HH12	1.57	0.70
1:B:361:LYS:HD2	4:B:722:HOH:O	1.91	0.70
1:A:429:ASP:HB2	4:A:717:HOH:O	1.91	0.70
1:C:147:LEU:HD23	1:C:179:LEU:HD23	1.73	0.70
1:C:136:ARG:HD3	4:C:718:HOH:O	1.91	0.70
1:C:246:GLY:C	1:C:249:LEU:HD13	2.11	0.70
1:A:188:GLY:CA	4:A:737:HOH:O	2.32	0.70
1:C:250:GLU:HG2	1:C:253:THR:HG22	1.74	0.70
1:D:310:LEU:HD13	4:D:704:HOH:O	1.92	0.69
1:D:437:ARG:HH21	1:D:440:PHE:CB	2.05	0.69
1:B:181:MET:O	1:B:184:GLN:NE2	2.18	0.69
1:D:437:ARG:NH2	1:D:440:PHE:C	2.43	0.69
1:D:540:GLY:O	1:D:563:PHE:CD2	2.45	0.69
1:C:437:ARG:CA	4:C:735:HOH:O	2.04	0.69
1:B:649:THR:HA	4:B:737:HOH:O	1.93	0.69
1:A:480:LYS:HB2	4:A:707:HOH:O	1.94	0.68
1:A:301:PHE:HB3	1:A:394:LEU:HG	1.76	0.68
1:C:187:THR:HG22	1:C:238:LEU:HD11	1.76	0.68
1:A:246:GLY:N	1:A:249:LEU:HD21	2.07	0.68
1:C:576:VAL:HA	4:C:701:HOH:O	1.93	0.68
1:C:310:LEU:H	1:C:310:LEU:HD13	1.57	0.68
1:D:177:GLU:HA	4:D:702:HOH:O	1.94	0.68
1:D:249:LEU:HD11	1:D:254:ARG:CZ	2.24	0.67
1:D:582:GLY:HA2	4:D:729:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:HA2	1:A:249:LEU:HD11	0.71	0.67
1:B:233:ASP:OD1	1:B:300:ARG:NH1	2.27	0.67
1:C:621:LYS:NZ	4:C:702:HOH:O	2.19	0.67
1:A:506:ILE:N	1:A:506:ILE:HD12	2.09	0.67
1:D:580:GLN:OE1	1:D:580:GLN:HA	1.95	0.67
1:D:637:ASP:HA	1:D:639:ARG:HH22	1.60	0.67
1:A:539:ILE:HD12	1:A:560:LEU:HD13	1.75	0.67
1:A:181:MET:O	1:A:184:GLN:HB2	1.95	0.67
2:N:2:DC:N4	3:M:20:DG:H1	1.91	0.67
1:A:249:LEU:CB	1:A:254:ARG:CZ	2.73	0.66
2:F:13:DG:C2'	2:F:14:DA:H5"	2.25	0.66
1:A:249:LEU:CD2	1:A:249:LEU:H	1.94	0.66
1:A:394:LEU:HD21	4:A:729:HOH:O	1.94	0.66
1:A:577:ILE:CG1	1:A:578:ARG:HB3	2.19	0.66
1:B:301:PHE:C	4:B:724:HOH:O	2.32	0.66
1:D:377:GLU:O	1:D:381:GLU:HG3	1.95	0.66
1:D:245:ALA:O	1:D:249:LEU:HD12	1.96	0.66
1:B:539:ILE:HD12	1:B:560:LEU:HD13	1.78	0.66
1:A:250:GLU:OE2	1:A:252:LYS:N	2.28	0.66
1:B:500:SER:HA	1:B:504:LYS:HB2	1.78	0.66
1:A:181:MET:SD	1:A:181:MET:N	2.69	0.66
1:D:542:ILE:HD11	1:D:562:ARG:HD2	1.77	0.66
1:C:148:ARG:NE	1:C:245:ALA:HB2	2.10	0.66
1:A:394:LEU:CD2	4:A:729:HOH:O	2.43	0.66
1:B:424:ALA:HB2	1:B:515:TRP:CD1	2.30	0.66
1:C:449:GLU:HB3	4:C:713:HOH:O	1.96	0.66
1:D:437:ARG:HE	1:D:441:VAL:H	1.43	0.66
1:D:381:GLU:CD	1:D:504:LYS:NZ	2.49	0.66
1:D:542:ILE:C	1:D:542:ILE:HD12	2.16	0.66
1:A:429:ASP:O	1:A:433:SER:OG	2.14	0.65
1:B:247:GLY:HA2	1:B:249:LEU:HD23	1.78	0.65
1:B:538:ILE:HA	4:B:710:HOH:O	1.96	0.65
1:D:633:GLN:HG2	1:D:634:MET:O	1.95	0.65
1:C:577:ILE:HG23	1:C:578:ARG:CD	2.27	0.65
1:D:378:SER:OG	1:D:381:GLU:OE2	2.09	0.65
2:F:13:DG:H5"	4:F:101:HOH:O	1.96	0.65
1:A:200:ARG:HD2	4:A:755:HOH:O	1.96	0.65
1:D:370:ARG:HD3	1:D:379:VAL:HG13	1.77	0.65
1:C:144:ILE:HB	1:C:183:LEU:HD12	1.79	0.64
1:B:540:GLY:O	1:B:563:PHE:CD2	2.50	0.64
1:C:493:GLN:CG	4:C:713:HOH:O	2.40	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HB2	4:A:716:HOH:O	1.96	0.64
1:C:370:ARG:NH1	1:C:412:VAL:O	2.26	0.64
1:D:128:LEU:O	1:D:131:LYS:HG2	1.98	0.64
1:C:577:ILE:HG23	1:C:578:ARG:HD3	1.79	0.64
1:C:437:ARG:CB	4:C:735:HOH:O	2.38	0.64
1:A:288:LYS:HB2	1:A:288:LYS:NZ	2.11	0.64
1:A:310:LEU:O	1:A:311:VAL:HG12	1.98	0.64
1:D:381:GLU:OE2	1:D:504:LYS:CE	2.45	0.64
1:C:127:GLU:O	1:C:131:LYS:HG2	1.98	0.64
1:C:612:LEU:O	4:C:702:HOH:O	2.14	0.64
1:B:127:GLU:HA	4:B:705:HOH:O	1.96	0.64
1:D:434:GLU:HB3	1:D:437:ARG:HB2	1.79	0.64
1:A:633:GLN:OE1	1:A:633:GLN:HA	1.99	0.63
1:A:310:LEU:CD2	1:A:312:ARG:H	2.12	0.63
1:D:213:ASN:ND2	1:D:427:LEU:HD12	2.12	0.63
1:B:379:VAL:HG12	2:F:6:DC:OP1	1.97	0.63
1:B:351:ILE:HD12	1:B:351:ILE:H	1.63	0.63
1:B:281:GLN:HB3	1:B:426:ILE:HG21	1.79	0.63
1:C:507:LEU:C	1:C:508:LEU:HD22	2.18	0.63
1:D:558:THR:O	1:D:576:VAL:HG22	1.99	0.63
1:A:249:LEU:CB	1:A:254:ARG:CD	2.77	0.63
1:A:252:LYS:HG3	1:A:253:THR:N	2.14	0.63
1:A:375:GLY:C	1:A:376:THR:HG23	2.19	0.63
1:C:387:LEU:HD11	1:C:404:GLN:HB2	1.80	0.63
1:A:310:LEU:H	1:A:310:LEU:CD1	2.12	0.62
1:C:315:MET:HG2	1:C:340:ILE:HD11	1.81	0.62
1:B:636:LYS:O	1:B:637:ASP:HB2	1.98	0.62
1:C:424:ALA:HB2	1:C:515:TRP:CD1	2.35	0.62
1:A:393:THR:H	1:A:400:PRO:HA	1.64	0.62
1:A:246:GLY:O	1:A:249:LEU:CD2	2.37	0.62
1:A:458:LYS:HE3	1:A:462:GLU:HG3	1.81	0.62
1:C:582:GLY:HA2	4:C:744:HOH:O	1.93	0.62
1:A:525:THR:HA	1:A:529:LEU:HB2	1.82	0.62
1:C:323:GLU:HA	1:C:324:LEU:HB2	1.81	0.62
1:A:540:GLY:O	1:A:563:PHE:CD2	2.53	0.62
1:D:542:ILE:HD11	1:D:547:VAL:CG1	2.30	0.62
1:C:246:GLY:O	1:C:249:LEU:HD13	1.99	0.61
1:B:637:ASP:HA	1:B:639:ARG:NH1	2.14	0.61
1:C:224:LEU:HD12	4:C:727:HOH:O	1.91	0.61
2:F:19:DC:H2"	2:F:20:DA:O4'	2.00	0.61
1:A:148:ARG:HD2	1:A:245:ALA:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLU:HG3	1:A:253:THR:HG23	1.82	0.61
1:B:637:ASP:OD1	1:B:638:GLY:HA2	2.01	0.61
1:C:247:GLY:H	1:C:249:LEU:HD13	1.65	0.61
1:C:250:GLU:HG2	1:C:250:GLU:O	2.00	0.61
1:A:249:LEU:HB2	1:A:254:ARG:NE	2.16	0.61
1:B:143:GLU:HB3	1:B:183:LEU:HD21	1.82	0.61
1:D:370:ARG:NH1	1:D:412:VAL:O	2.34	0.61
1:D:633:GLN:O	1:D:634:MET:HB2	2.01	0.61
1:D:381:GLU:OE1	1:D:504:LYS:NZ	2.34	0.61
1:C:273:PHE:CD1	4:C:717:HOH:O	2.49	0.61
1:B:542:ILE:HD11	1:B:546:TYR:HD2	1.65	0.60
1:A:250:GLU:CD	1:A:251:PRO:N	2.49	0.60
1:B:587:GLU:OE1	1:D:636:LYS:NZ	2.34	0.60
1:D:128:LEU:HA	1:D:131:LYS:HD3	1.83	0.60
1:C:214:GLY:HA3	1:C:461:ALA:HB2	1.83	0.60
1:A:311:VAL:HG13	1:A:311:VAL:O	2.01	0.60
1:A:395:GLY:HA2	1:A:397:GLY:N	2.17	0.60
1:C:223:PRO:HG2	4:C:727:HOH:O	2.02	0.60
1:D:190:LEU:HD23	1:D:234:ILE:HD11	1.82	0.60
1:B:347:LEU:HA	1:B:358:ALA:HB2	1.82	0.60
1:A:499:TRP:CZ2	4:A:747:HOH:O	2.51	0.60
1:B:307:LYS:HG3	1:B:308:PRO:HD2	1.83	0.60
1:C:213:ASN:HA	1:C:458:LYS:HD3	1.83	0.59
1:D:398:LYS:HB3	1:D:400:PRO:HG3	1.83	0.59
1:D:601:SER:HB2	4:D:717:HOH:O	2.02	0.59
1:A:249:LEU:CB	1:A:254:ARG:NE	2.64	0.59
1:A:467:ARG:CG	4:A:746:HOH:O	2.50	0.59
1:D:132:THR:HA	1:D:135:ARG:HG3	1.84	0.59
1:B:127:GLU:HG2	1:B:227:ARG:NH1	2.17	0.59
1:D:612:LEU:HD22	1:D:612:LEU:H	1.67	0.59
1:A:596:ASP:O	1:A:605:ARG:NH2	2.30	0.59
1:D:179:LEU:HD21	1:D:182:LEU:HD22	0.65	0.59
1:D:437:ARG:HG2	1:D:438:VAL:N	2.17	0.59
1:B:286:GLN:HA	1:B:364:LEU:HD21	1.83	0.59
1:A:233:ASP:OD1	1:A:300:ARG:NH1	2.35	0.59
1:A:578:ARG:CZ	1:A:582:GLY:HA3	2.32	0.59
1:C:136:ARG:CD	4:C:718:HOH:O	2.50	0.59
1:A:420:ASN:HA	1:A:423:LYS:HE3	1.84	0.59
1:C:148:ARG:HB3	4:C:746:HOH:O	2.03	0.59
1:D:177:GLU:HB3	4:D:702:HOH:O	2.03	0.59
1:C:147:LEU:HG	1:C:179:LEU:HG	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:538:ILE:HG22	1:C:540:GLY:N	2.18	0.59
1:D:202:GLN:CG	4:D:730:HOH:O	2.51	0.59
1:C:275:VAL:CB	4:C:722:HOH:O	2.51	0.58
1:B:630:LYS:HG2	1:B:631:PRO:HD2	1.84	0.58
1:D:437:ARG:NH2	1:D:440:PHE:HB3	2.17	0.58
1:A:538:ILE:HG22	1:A:540:GLY:CA	2.33	0.58
1:C:131:LYS:O	1:C:135:ARG:HG2	2.04	0.58
1:C:507:LEU:HB2	1:C:508:LEU:HD23	1.84	0.58
1:D:542:ILE:HD13	1:D:543:SER:O	2.03	0.58
1:B:525:THR:HA	1:B:529:LEU:HB2	1.85	0.58
1:A:499:TRP:CE2	4:A:747:HOH:O	2.55	0.58
2:F:20:DA:H3'	2:F:21:DT:H4'	1.86	0.58
1:A:249:LEU:HD23	1:A:249:LEU:N	2.02	0.58
1:B:183:LEU:O	1:B:187:THR:OG1	2.12	0.58
1:B:311:VAL:HG12	1:B:390:ALA:HB2	1.85	0.58
1:A:250:GLU:O	1:A:254:ARG:HG2	2.04	0.58
1:A:527:ARG:CD	4:A:702:HOH:O	2.51	0.58
1:D:458:LYS:HE3	1:D:462:GLU:HG3	1.86	0.58
1:B:587:GLU:CD	1:D:636:LYS:HZ3	2.06	0.58
1:D:628:HIS:CD2	4:D:723:HOH:O	2.37	0.58
1:A:188:GLY:HA3	1:A:260:ARG:HH21	1.68	0.58
1:A:254:ARG:O	1:A:258:THR:OG1	2.21	0.58
1:C:148:ARG:HH21	1:C:245:ALA:N	2.00	0.58
1:C:609:LEU:O	4:C:702:HOH:O	2.17	0.58
1:D:179:LEU:HD21	1:D:182:LEU:CG	2.16	0.58
1:D:370:ARG:HD3	1:D:379:VAL:CG1	2.33	0.57
1:B:621:LYS:HG3	1:B:622:ASP:N	2.18	0.57
1:A:126:GLU:OE1	1:A:200:ARG:NH2	2.33	0.57
1:B:224:LEU:HD23	4:B:725:HOH:O	2.05	0.57
1:C:323:GLU:CB	4:C:733:HOH:O	2.51	0.57
1:C:381:GLU:CD	1:C:504:LYS:HZ2	1.99	0.57
1:D:392:PHE:CE1	1:D:401:ILE:HD11	2.39	0.57
1:A:179:LEU:O	1:A:182:LEU:HB3	2.04	0.57
1:C:181:MET:O	1:C:184:GLN:HG3	2.04	0.57
1:D:212:GLY:O	1:D:213:ASN:HB2	2.05	0.57
1:D:234:ILE:HA	1:D:237:GLN:HG3	1.87	0.57
1:A:131:LYS:O	1:A:135:ARG:HG2	2.05	0.57
1:C:377:GLU:HB2	1:C:378:SER:HB2	1.87	0.57
2:F:12:DG:H2"	4:F:101:HOH:O	2.05	0.57
1:B:254:ARG:O	1:B:258:THR:OG1	2.21	0.56
1:D:578:ARG:HB3	1:D:578:ARG:CZ	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:600:ARG:HG2	1:D:605:ARG:HG3	1.87	0.56
1:C:420:ASN:HB2	4:C:714:HOH:O	2.05	0.56
1:D:501:GLN:HA	1:D:505:GLU:HG2	1.86	0.56
1:C:379:VAL:HG11	3:M:6:DT:H3'	1.86	0.56
1:A:609:LEU:HB2	1:A:612:LEU:HD11	1.87	0.56
1:C:402:GLN:H	1:C:402:GLN:CD	2.07	0.56
1:D:324:LEU:CB	4:D:728:HOH:O	2.41	0.56
1:D:378:SER:C	1:D:379:VAL:HG23	2.24	0.56
1:A:219:GLU:OE2	1:A:219:GLU:N	2.38	0.56
1:A:467:ARG:CB	4:A:733:HOH:O	2.22	0.56
1:D:500:SER:HA	1:D:504:LYS:HB2	1.86	0.56
1:A:246:GLY:CA	1:A:249:LEU:CD1	2.38	0.56
1:A:310:LEU:N	1:A:310:LEU:HD13	2.20	0.56
1:B:370:ARG:NH1	1:B:412:VAL:O	2.37	0.56
1:C:379:VAL:CB	4:C:732:HOH:O	2.54	0.56
1:B:138:GLN:NE2	4:B:704:HOH:O	2.38	0.56
1:B:310:LEU:HD12	1:B:344:THR:HG22	1.87	0.56
1:B:323:GLU:HA	1:B:324:LEU:HB2	1.86	0.56
1:D:636:LYS:C	1:D:639:ARG:HH12	2.09	0.56
1:A:148:ARG:HD2	1:A:245:ALA:HB3	1.87	0.56
1:C:638:GLY:O	4:C:703:HOH:O	2.18	0.56
1:D:126:GLU:O	1:D:129:LYS:HG2	2.04	0.56
1:D:212:GLY:O	1:D:213:ASN:CB	2.53	0.56
1:C:275:VAL:CG2	4:C:722:HOH:O	2.44	0.56
1:A:347:LEU:HA	1:A:358:ALA:HB2	1.88	0.55
1:C:440:PHE:CE1	4:C:739:HOH:O	2.47	0.55
1:D:370:ARG:HH11	1:D:412:VAL:HG13	1.71	0.55
1:A:506:ILE:HG22	1:A:507:LEU:O	2.06	0.55
1:B:561:LEU:HB2	4:B:710:HOH:O	2.06	0.55
1:C:376:THR:HG21	4:C:724:HOH:O	2.03	0.55
1:D:424:ALA:HB2	1:D:515:TRP:CD1	2.41	0.55
1:A:472:GLU:HG2	4:A:728:HOH:O	2.07	0.55
1:B:130:PHE:CE2	1:B:227:ARG:HD2	2.41	0.55
1:B:542:ILE:HD11	1:B:546:TYR:CD2	2.41	0.55
1:B:646:ILE:HD13	4:D:715:HOH:O	2.06	0.55
1:B:213:ASN:HD22	1:B:427:LEU:CD1	2.13	0.55
1:B:632:GLU:H	1:B:632:GLU:CD	2.04	0.55
1:C:249:LEU:HD12	1:C:249:LEU:N	2.22	0.55
1:D:184:GLN:O	1:D:187:THR:HG23	2.07	0.55
1:D:437:ARG:NE	1:D:441:VAL:N	2.47	0.55
1:A:527:ARG:NE	4:A:702:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLU:HG3	4:B:701:HOH:O	2.06	0.55
1:B:398:LYS:HB3	1:B:400:PRO:HD3	1.89	0.55
1:C:298:GLY:O	1:C:349:ASN:ND2	2.39	0.55
1:A:449:GLU:HG3	1:A:450:LYS:N	2.22	0.55
1:B:366:LYS:O	1:B:366:LYS:HD3	2.06	0.55
1:D:188:GLY:O	1:D:191:GLU:HG2	2.06	0.55
1:A:500:SER:O	1:A:505:GLU:N	2.39	0.54
1:B:493:GLN:HG3	4:B:745:HOH:O	2.07	0.54
4:A:751:HOH:O	1:C:646:ILE:CD1	2.56	0.54
1:B:260:ARG:O	1:B:264:VAL:HG13	2.06	0.54
1:B:250:GLU:HG2	1:B:251:PRO:HD2	1.88	0.54
1:B:315:MET:HG2	1:B:340:ILE:HD11	1.90	0.54
1:C:616:TYR:CD1	1:C:617:PRO:HB3	2.42	0.54
1:C:442:VAL:HA	4:C:716:HOH:O	2.07	0.54
1:D:179:LEU:HD23	1:D:182:LEU:CD1	2.38	0.54
1:D:341:ILE:HG12	1:D:364:LEU:HB3	1.90	0.54
1:D:538:ILE:HG22	1:D:540:GLY:N	2.23	0.54
1:B:200:ARG:NH2	4:B:705:HOH:O	2.40	0.54
1:C:188:GLY:O	1:C:191:GLU:HG2	2.07	0.54
1:D:621:LYS:HG3	1:D:622:ASP:N	2.22	0.54
1:C:294:ARG:NH2	1:C:355:CYS:HB3	2.23	0.54
1:D:180:ALA:HA	1:D:183:LEU:N	2.22	0.54
3:M:18:DC:H2"	3:M:19:DA:C8	2.43	0.54
1:A:221:LEU:HA	4:A:716:HOH:O	2.08	0.54
1:C:141:VAL:HA	1:C:144:ILE:HG22	1.89	0.54
1:C:323:GLU:HB2	4:C:733:HOH:O	2.08	0.54
1:D:578:ARG:HG2	1:D:579:GLY:O	2.08	0.54
1:B:140:ARG:HD2	1:B:183:LEU:HD11	1.89	0.53
1:D:367:LYS:CE	1:D:367:LYS:CA	2.30	0.53
1:C:622:ASP:O	1:C:626:ARG:HG2	2.08	0.53
1:D:323:GLU:HA	1:D:324:LEU:HB2	1.90	0.53
1:C:190:LEU:CG	4:C:737:HOH:O	2.52	0.53
1:D:539:ILE:HG21	1:D:542:ILE:CG2	2.38	0.53
1:C:307:LYS:NZ	1:C:307:LYS:HA	2.23	0.53
1:D:180:ALA:CB	4:D:719:HOH:O	2.56	0.53
1:C:126:GLU:OE1	1:C:227:ARG:NH2	2.41	0.53
1:D:506:ILE:CG2	4:D:706:HOH:O	2.46	0.53
2:N:21:DT:C4	3:M:1:DA:N6	2.77	0.53
1:C:392:PHE:CD1	1:C:394:LEU:HB2	2.43	0.53
1:C:179:LEU:HD13	1:C:180:ALA:N	2.24	0.53
2:F:12:DG:H2"	2:F:13:DG:C8	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:557:GLY:O	1:D:613:LYS:N	2.41	0.53
1:D:324:LEU:HD13	4:D:728:HOH:O	2.08	0.53
2:N:20:DA:H1'	2:N:21:DT:O4'	2.09	0.53
1:A:141:VAL:HA	1:A:144:ILE:HG22	1.91	0.52
1:C:392:PHE:HA	1:C:393:THR:OG1	2.09	0.52
1:A:249:LEU:CD1	1:A:254:ARG:HG3	2.27	0.52
1:A:542:ILE:HG23	1:A:562:ARG:NE	2.23	0.52
1:B:322:ARG:N	4:B:701:HOH:O	2.42	0.52
1:C:393:THR:H	1:C:400:PRO:HA	1.74	0.52
1:D:542:ILE:CD1	1:D:543:SER:O	2.57	0.52
1:A:138:GLN:O	1:A:141:VAL:HG12	2.10	0.52
1:A:127:GLU:O	1:A:131:LYS:HG2	2.09	0.52
1:A:310:LEU:C	1:A:310:LEU:HD22	2.30	0.52
1:C:436:ASP:OD1	1:C:436:ASP:N	2.42	0.52
1:D:615:LEU:N	1:D:619:LYS:O	2.41	0.52
1:A:310:LEU:N	1:A:310:LEU:CD1	2.73	0.52
1:B:280:PRO:HG2	1:B:283:LEU:HD13	1.91	0.52
1:C:125:GLN:O	1:C:129:LYS:HG2	2.10	0.52
1:C:542:ILE:HG12	1:C:543:SER:N	2.24	0.52
1:D:203:ILE:HG13	1:D:435:MET:HE1	1.92	0.52
1:A:398:LYS:H	1:A:398:LYS:HD2	1.74	0.52
1:C:542:ILE:CD1	1:C:547:VAL:CG1	2.59	0.52
1:D:542:ILE:HD12	1:D:543:SER:C	2.30	0.52
1:B:463:VAL:O	1:B:530:ARG:HD3	2.10	0.52
1:B:634:MET:CG	1:B:635:GLY:N	2.73	0.52
1:D:179:LEU:HD22	1:D:182:LEU:CD2	2.32	0.52
1:A:286:GLN:HA	1:A:364:LEU:HD21	1.92	0.52
1:A:557:GLY:O	1:A:613:LYS:N	2.42	0.52
1:B:310:LEU:CD1	1:B:344:THR:HG22	2.39	0.52
1:C:508:LEU:CD2	1:C:508:LEU:N	2.73	0.52
1:D:148:ARG:NH1	1:D:241:GLU:OE1	2.43	0.52
1:D:399:LEU:N	1:D:400:PRO:HD3	2.25	0.52
1:A:398:LYS:N	1:A:398:LYS:HD2	2.25	0.51
1:B:250:GLU:OE2	1:B:252:LYS:N	2.28	0.51
1:B:519:ASP:HA	1:B:522:LEU:HB2	1.93	0.51
1:C:376:THR:HG22	4:C:712:HOH:O	2.10	0.51
1:C:266:ARG:HD3	4:C:747:HOH:O	2.07	0.51
1:C:525:THR:HA	1:C:529:LEU:HB2	1.92	0.51
1:C:299:LEU:HB2	4:C:704:HOH:O	2.10	0.51
1:A:188:GLY:HA3	1:A:260:ARG:NH2	2.25	0.51
1:B:361:LYS:H	1:B:361:LYS:HD2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ASP:CG	4:C:725:HOH:O	2.48	0.51
1:C:394:LEU:HD21	4:C:738:HOH:O	2.03	0.51
1:D:204:TRP:CE2	1:D:221:LEU:HD13	2.46	0.51
1:D:228:CYS:HB3	1:D:297:LEU:HD21	1.92	0.51
1:D:367:LYS:HD3	1:D:368:ILE:H	1.75	0.51
2:N:12:DG:H2"	2:N:13:DG:C8	2.45	0.51
2:N:20:DA:C4	2:N:21:DT:O2	2.63	0.51
1:A:311:VAL:HG11	1:A:358:ALA:HB1	1.92	0.51
1:B:233:ASP:O	1:B:237:GLN:HG3	2.11	0.51
1:C:214:GLY:HA3	1:C:461:ALA:CB	2.41	0.51
1:C:249:LEU:CD1	1:C:249:LEU:N	2.73	0.51
1:C:376:THR:OG1	1:C:377:GLU:N	2.40	0.51
1:B:127:GLU:O	1:B:130:PHE:HB3	2.11	0.51
1:B:378:SER:O	1:B:381:GLU:HG2	2.11	0.51
1:D:177:GLU:N	4:D:702:HOH:O	2.43	0.51
1:C:260:ARG:O	1:C:264:VAL:HG13	2.10	0.51
1:D:260:ARG:O	1:D:264:VAL:HG13	2.10	0.51
1:D:495:ARG:HD3	4:D:711:HOH:O	2.11	0.51
1:A:424:ALA:HB2	1:A:515:TRP:CD1	2.46	0.51
1:B:392:PHE:HA	1:B:393:THR:OG1	2.10	0.51
1:A:310:LEU:HD22	1:A:312:ARG:H	1.76	0.50
1:A:584:PRO:CG	4:A:759:HOH:O	2.59	0.50
1:A:513:THR:HB	4:A:722:HOH:O	2.11	0.50
1:B:556:ASP:OD1	1:B:577:ILE:HA	2.10	0.50
1:A:178:ALA:N	4:A:705:HOH:O	2.45	0.50
1:A:542:ILE:HG22	1:A:562:ARG:CB	2.40	0.50
1:D:179:LEU:CD2	1:D:182:LEU:CD1	2.89	0.50
1:D:249:LEU:HD21	1:D:254:ARG:HH12	1.76	0.50
1:A:544:LYS:O	1:A:547:VAL:HG22	2.11	0.50
1:B:429:ASP:OD2	1:B:437:ARG:NH2	2.45	0.50
1:C:130:PHE:CE2	1:C:227:ARG:HD2	2.47	0.50
1:A:322:ARG:O	1:A:324:LEU:HB2	2.11	0.50
1:A:636:LYS:O	1:A:639:ARG:NH1	2.44	0.50
1:B:395:GLY:HA2	1:B:396:PRO:C	2.31	0.50
1:B:538:ILE:HG22	1:B:540:GLY:CA	2.41	0.50
1:B:544:LYS:O	1:B:547:VAL:HG22	2.10	0.50
1:D:503:ASN:O	1:D:513:THR:HG21	2.12	0.50
3:E:20:DG:N2	2:F:3:DT:O2	2.44	0.50
1:A:213:ASN:ND2	1:A:427:LEU:HD12	2.26	0.50
1:A:130:PHE:CE2	1:A:227:ARG:HD2	2.46	0.50
1:A:542:ILE:CG2	1:A:562:ARG:NE	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:ALA:O	1:D:184:GLN:HG2	2.12	0.50
1:D:249:LEU:O	1:D:249:LEU:HD13	2.12	0.50
1:C:359:LEU:N	4:C:706:HOH:O	2.45	0.50
1:C:213:ASN:HA	1:C:458:LYS:CD	2.41	0.50
1:A:361:LYS:HD2	1:A:361:LYS:H	1.77	0.50
1:D:151:LEU:HB3	1:D:248:GLU:OE2	2.12	0.50
2:F:20:DA:H2'	2:F:20:DA:N3	2.27	0.50
1:B:596:ASP:O	1:B:605:ARG:NH2	2.43	0.49
1:A:350:SER:HB2	4:A:753:HOH:O	2.12	0.49
1:A:506:ILE:N	1:A:506:ILE:CD1	2.73	0.49
1:D:377:GLU:O	1:D:381:GLU:CG	2.59	0.49
1:A:467:ARG:HG2	4:A:746:HOH:O	2.12	0.49
1:C:140:ARG:NH2	4:C:707:HOH:O	2.45	0.49
1:D:572:THR:OG1	1:D:589:ILE:O	2.20	0.49
1:B:298:GLY:HA3	1:B:356:CYS:CB	2.42	0.49
1:C:252:LYS:HD3	1:C:253:THR:N	2.28	0.49
1:A:246:GLY:HA2	1:A:249:LEU:CD2	2.35	0.49
1:B:417:ASN:OD1	1:B:418:GLN:HG3	2.12	0.49
1:D:217:PHE:HB3	1:D:219:GLU:HG2	1.95	0.49
1:A:134:LEU:HD11	1:A:230:SER:HB3	1.93	0.49
1:D:544:LYS:O	1:D:547:VAL:HG22	2.12	0.49
1:B:251:PRO:O	1:B:254:ARG:HB3	2.13	0.49
1:B:626:ARG:NH2	4:B:707:HOH:O	2.45	0.49
1:C:306:ALA:HB3	4:C:738:HOH:O	2.13	0.49
1:C:577:ILE:CD1	1:C:611:GLN:HB2	2.40	0.49
1:D:388:PHE:O	1:D:404:GLN:HA	2.12	0.49
1:C:250:GLU:N	1:C:251:PRO:HD3	2.27	0.49
1:C:393:THR:HG22	1:C:400:PRO:HB3	1.93	0.49
3:E:16:DG:H2"	3:E:17:DA:C8	2.47	0.49
1:B:577:ILE:HD13	1:B:585:GLN:O	2.12	0.49
1:D:525:THR:HA	1:D:529:LEU:HB2	1.94	0.49
1:A:527:ARG:HG2	4:A:702:HOH:O	2.12	0.48
1:B:309:PRO:O	1:B:310:LEU:HG	2.12	0.48
1:C:485:ASN:OD1	1:C:485:ASN:N	2.46	0.48
1:D:379:VAL:CG2	3:E:6:DT:OP1	2.49	0.48
1:C:213:ASN:OD1	1:C:213:ASN:N	2.47	0.48
1:C:398:LYS:HB2	1:C:400:PRO:HD3	1.95	0.48
1:D:361:LYS:N	4:D:708:HOH:O	2.46	0.48
1:D:439:PRO:HA	1:D:440:PHE:HA	1.64	0.48
1:C:368:ILE:HD13	1:C:369:LYS:N	2.28	0.48
1:A:146:LEU:O	1:A:149:GLU:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LEU:CD1	4:A:727:HOH:O	2.53	0.48
1:A:261:LEU:O	1:A:264:VAL:HG22	2.12	0.48
1:A:542:ILE:HG13	1:A:543:SER:H	1.78	0.48
1:B:392:PHE:CD1	1:B:394:LEU:HB3	2.49	0.48
1:C:148:ARG:HH21	1:C:245:ALA:CA	2.27	0.48
1:A:459:PHE:HA	1:A:522:LEU:HD11	1.93	0.48
1:B:193:ALA:O	1:B:197:VAL:HG12	2.14	0.48
1:C:252:LYS:HD3	1:C:252:LYS:C	2.34	0.48
1:D:179:LEU:CD2	1:D:182:LEU:HD13	2.43	0.48
1:B:127:GLU:OE1	1:B:131:LYS:HE3	2.13	0.48
1:C:250:GLU:CG	1:C:253:THR:CG2	2.91	0.48
1:C:398:LYS:HZ2	1:C:398:LYS:N	2.11	0.48
1:D:249:LEU:HD21	1:D:254:ARG:HH22	1.77	0.48
1:D:539:ILE:HG21	1:D:542:ILE:HG21	1.95	0.48
1:A:234:ILE:HG13	1:A:235:TYR:N	2.28	0.48
1:A:434:GLU:O	1:A:434:GLU:HG3	2.12	0.48
1:B:127:GLU:CA	4:B:705:HOH:O	2.57	0.48
1:B:379:VAL:HG12	2:F:6:DC:P	2.54	0.48
1:C:376:THR:CG2	4:C:712:HOH:O	2.60	0.48
1:C:392:PHE:HD1	1:C:394:LEU:HB2	1.78	0.48
1:D:503:ASN:O	1:D:503:ASN:ND2	2.46	0.48
1:A:351:ILE:H	1:A:351:ILE:HD12	1.78	0.48
1:B:551:LEU:HB3	1:B:576:VAL:CG2	2.43	0.48
1:C:249:LEU:CD1	1:C:249:LEU:H	2.27	0.48
1:C:269:VAL:HG12	1:C:297:LEU:HD13	1.96	0.48
1:A:387:LEU:HD11	1:A:404:GLN:HB2	1.95	0.48
1:B:469:LEU:HD22	1:B:541:PHE:CE2	2.48	0.47
1:C:558:THR:O	1:C:576:VAL:HG12	2.13	0.47
1:D:370:ARG:HD2	3:E:7:DT:OP1	2.14	0.47
1:D:485:ASN:OD1	1:D:485:ASN:N	2.46	0.47
3:E:11:DT:H2"	3:E:12:DG:C8	2.49	0.47
1:A:637:ASP:CG	1:A:639:ARG:HH22	2.18	0.47
1:B:350:SER:CB	4:B:740:HOH:O	2.51	0.47
1:D:215:ALA:O	1:D:216:PRO:C	2.51	0.47
1:A:250:GLU:OE2	1:A:251:PRO:HD2	1.65	0.47
1:B:221:LEU:HA	4:B:725:HOH:O	2.13	0.47
1:C:507:LEU:HB2	1:C:508:LEU:HD22	1.92	0.47
1:D:575:HIS:CE1	1:D:587:GLU:HB2	2.48	0.47
1:A:375:GLY:O	1:A:376:THR:HG23	2.14	0.47
1:B:138:GLN:O	1:B:141:VAL:HG12	2.14	0.47
1:B:234:ILE:HG13	1:B:235:TYR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HA	1:B:345:VAL:O	2.14	0.47
1:B:323:GLU:N	4:B:701:HOH:O	2.41	0.47
1:B:587:GLU:CB	4:B:719:HOH:O	2.63	0.47
1:D:312:ARG:HA	1:D:343:ASN:O	2.14	0.47
1:D:406:LEU:HA	1:D:406:LEU:HD12	1.73	0.47
2:F:19:DC:C2	2:F:20:DA:H8	2.33	0.47
1:A:199:LYS:O	1:A:203:ILE:HD12	2.15	0.47
1:A:246:GLY:O	1:A:249:LEU:CD1	2.54	0.47
1:B:392:PHE:HD1	1:B:394:LEU:HB3	1.79	0.47
1:C:275:VAL:HG11	4:C:722:HOH:O	2.14	0.47
1:D:140:ARG:HE	1:D:186:THR:HB	1.78	0.47
1:D:367:LYS:CD	1:D:368:ILE:H	2.27	0.47
1:C:126:GLU:HG2	1:C:126:GLU:O	2.15	0.47
1:C:388:PHE:O	1:C:404:GLN:HA	2.15	0.47
1:C:433:SER:OG	1:C:437:ARG:CZ	2.63	0.47
1:C:577:ILE:HG23	1:C:578:ARG:HD2	1.97	0.47
1:D:505:GLU:O	1:D:505:GLU:HG3	2.15	0.47
1:B:140:ARG:HD3	1:B:140:ARG:HA	1.59	0.47
1:C:395:GLY:HA2	1:C:396:PRO:C	2.35	0.47
1:A:215:ALA:HB1	1:A:216:PRO:HD2	1.97	0.47
1:A:471:PRO:HB2	4:A:728:HOH:O	2.14	0.47
1:B:366:LYS:HD2	1:B:367:LYS:N	2.26	0.47
1:D:636:LYS:CB	1:D:639:ARG:HH12	2.24	0.47
1:B:307:LYS:HA	1:B:307:LYS:HE2	1.96	0.46
1:C:185:GLU:HA	1:C:185:GLU:OE2	2.14	0.46
1:C:266:ARG:HD2	4:C:747:HOH:O	2.09	0.46
1:D:179:LEU:HD22	1:D:182:LEU:HD22	1.76	0.46
1:D:578:ARG:HG2	1:D:579:GLY:N	2.29	0.46
1:A:148:ARG:HD2	1:A:245:ALA:HB2	1.97	0.46
1:C:136:ARG:HG2	4:C:718:HOH:O	2.14	0.46
1:C:254:ARG:O	1:C:257:LEU:HB2	2.15	0.46
1:B:637:ASP:CA	1:B:639:ARG:HH12	2.27	0.46
1:C:307:LYS:HA	1:C:307:LYS:HZ3	1.80	0.46
1:C:575:HIS:CE1	1:C:587:GLU:HB2	2.50	0.46
1:A:249:LEU:HB2	1:A:254:ARG:HG3	1.94	0.46
1:B:310:LEU:CA	1:B:346:PRO:HA	2.36	0.46
1:D:180:ALA:HB1	4:D:719:HOH:O	2.16	0.46
1:D:179:LEU:O	1:D:180:ALA:HB3	2.15	0.46
1:D:180:ALA:CA	1:D:183:LEU:HB2	2.24	0.46
1:D:280:PRO:HG2	1:D:283:LEU:HD12	1.98	0.46
1:B:398:LYS:O	4:B:702:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLN:O	1:C:141:VAL:HG12	2.16	0.46
1:C:247:GLY:H	1:C:249:LEU:CD1	2.27	0.46
1:C:341:ILE:HG12	1:C:364:LEU:HB3	1.97	0.46
1:B:638:GLY:HA2	1:B:639:ARG:HA	1.63	0.46
1:C:251:PRO:O	1:C:254:ARG:HB3	2.15	0.46
1:C:319:LYS:N	4:C:710:HOH:O	2.48	0.46
1:D:125:GLN:O	1:D:129:LYS:NZ	2.39	0.46
1:D:622:ASP:O	1:D:626:ARG:HG2	2.16	0.46
1:D:638:GLY:HA2	1:D:639:ARG:HA	1.67	0.46
1:A:398:LYS:HB3	4:A:741:HOH:O	2.14	0.46
1:C:363:LEU:HA	1:C:363:LEU:HD12	1.75	0.46
3:E:20:DG:H2"	3:E:21:DA:C8	2.51	0.46
2:F:13:DG:H8	4:F:101:HOH:O	1.99	0.46
2:F:13:DG:H2"	2:F:14:DA:H5"	1.96	0.46
1:B:223:PRO:O	1:B:227:ARG:HG2	2.15	0.46
1:D:130:PHE:CE2	1:D:227:ARG:HD2	2.51	0.46
1:D:307:LYS:HA	1:D:307:LYS:HD2	1.73	0.46
1:A:392:PHE:HA	1:A:393:THR:OG1	2.16	0.46
1:A:503:ASN:O	1:A:513:THR:HG21	2.16	0.46
1:B:600:ARG:HG2	1:B:605:ARG:HG3	1.98	0.46
1:C:507:LEU:N	1:C:507:LEU:CD1	2.73	0.46
1:D:558:THR:HA	1:D:614:ASN:O	2.16	0.46
1:A:542:ILE:HG13	1:A:543:SER:N	2.31	0.45
1:C:543:SER:O	1:C:547:VAL:HG13	2.15	0.45
1:D:378:SER:O	1:D:380:THR:HG23	2.15	0.45
1:B:191:GLU:HG2	1:B:264:VAL:HG11	1.97	0.45
1:D:188:GLY:HA2	1:D:191:GLU:HG2	1.98	0.45
1:D:250:GLU:O	1:D:253:THR:OG1	2.34	0.45
1:D:301:PHE:HD2	1:D:392:PHE:HE2	1.63	0.45
1:D:484:ASP:HB3	1:D:492:PHE:CE1	2.51	0.45
1:D:637:ASP:HA	1:D:639:ARG:NH2	2.28	0.45
1:B:551:LEU:HB3	1:B:576:VAL:HG22	1.97	0.45
1:B:622:ASP:O	1:B:626:ARG:HG2	2.16	0.45
1:C:437:ARG:HD3	1:C:438:VAL:O	2.15	0.45
1:C:136:ARG:CG	4:C:718:HOH:O	2.64	0.45
1:C:379:VAL:CA	4:C:732:HOH:O	2.64	0.45
1:D:576:VAL:HG12	1:D:586:ILE:HD12	1.98	0.45
1:A:228:CYS:HB3	1:A:297:LEU:HD21	1.97	0.45
1:A:476:PHE:CE1	1:A:542:ILE:O	2.69	0.45
1:D:607:ARG:HB2	1:D:629:TYR:CE1	2.52	0.45
1:B:517:TRP:HA	1:B:568:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:VAL:CG1	4:C:732:HOH:O	2.30	0.45
1:C:577:ILE:HG12	1:C:578:ARG:HH11	1.82	0.45
1:D:144:ILE:HD11	1:D:241:GLU:HB3	1.99	0.45
1:D:310:LEU:HD11	4:D:704:HOH:O	2.11	0.45
1:D:541:PHE:CD1	1:D:541:PHE:N	2.85	0.45
1:D:551:LEU:HB3	1:D:576:VAL:CG1	2.47	0.45
3:E:14:DA:H2"	3:E:15:DA:C8	2.51	0.45
2:N:21:DT:O4	3:M:1:DA:C6	2.69	0.45
1:D:437:ARG:HG2	1:D:438:VAL:O	2.16	0.45
1:D:617:PRO:CA	4:D:707:HOH:O	2.49	0.45
2:N:20:DA:H2"	2:N:21:DT:O5'	2.17	0.45
1:A:476:PHE:CD2	1:A:541:PHE:HB3	2.51	0.45
1:B:587:GLU:HB3	4:B:719:HOH:O	2.17	0.45
1:C:180:ALA:CB	1:C:250:GLU:OE1	2.61	0.45
1:D:212:GLY:C	1:D:213:ASN:OD1	2.56	0.45
1:A:249:LEU:CB	1:A:254:ARG:HD2	2.47	0.44
1:B:252:LYS:HG3	1:B:253:THR:N	2.32	0.44
1:B:637:ASP:CB	1:B:639:ARG:HH12	2.23	0.44
1:C:223:PRO:O	1:C:227:ARG:HG2	2.16	0.44
1:C:310:LEU:O	1:C:310:LEU:HD22	2.17	0.44
1:C:638:GLY:HA2	1:C:639:ARG:HA	1.60	0.44
1:D:295:PHE:O	1:D:356:CYS:HB3	2.17	0.44
3:E:20:DG:N2	4:E:101:HOH:O	2.50	0.44
1:A:184:GLN:HB3	1:A:257:LEU:HD11	2.00	0.44
1:A:392:PHE:CD1	1:A:394:LEU:HB2	2.52	0.44
1:A:584:PRO:HG3	4:A:759:HOH:O	2.16	0.44
1:B:125:GLN:HG2	4:B:751:HOH:O	2.06	0.44
1:B:587:GLU:HG3	4:B:719:HOH:O	2.16	0.44
1:D:322:ARG:HA	1:D:439:PRO:HG2	1.99	0.44
3:E:1:DA:H2"	3:E:2:DT:H5'	2.00	0.44
1:A:402:GLN:CD	1:A:402:GLN:H	2.21	0.44
1:C:607:ARG:HB2	1:C:629:TYR:CE1	2.52	0.44
1:D:202:GLN:HG3	4:D:730:HOH:O	2.15	0.44
1:D:230:SER:O	1:D:233:ASP:HB2	2.17	0.44
1:D:395:GLY:HA2	1:D:396:PRO:C	2.38	0.44
1:D:533:TRP:HA	4:D:705:HOH:O	2.17	0.44
1:A:260:ARG:O	1:A:264:VAL:HG13	2.17	0.44
1:A:634:MET:HG3	1:A:635:GLY:N	2.33	0.44
1:C:600:ARG:NH1	1:C:604:ASP:HB3	2.32	0.44
1:B:439:PRO:HA	1:B:440:PHE:HA	1.59	0.44
1:B:583:SER:OG	1:B:584:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:ARG:C	1:D:301:PHE:HD1	2.21	0.44
1:A:542:ILE:HD11	1:A:546:TYR:HD2	1.82	0.44
1:A:561:LEU:HB2	4:A:723:HOH:O	2.18	0.44
1:B:579:GLY:C	1:B:580:GLN:CG	2.86	0.44
1:D:581:ASP:OD1	1:D:582:GLY:N	2.50	0.44
2:F:12:DG:C2'	4:F:101:HOH:O	2.62	0.44
1:B:261:LEU:O	1:B:264:VAL:HG22	2.17	0.44
1:C:616:TYR:HA	1:C:617:PRO:HA	1.54	0.44
1:D:148:ARG:HE	1:D:148:ARG:C	2.21	0.44
1:A:307:LYS:HG3	1:A:308:PRO:HD2	1.98	0.44
1:A:617:PRO:HG2	1:A:618:LYS:HE2	1.99	0.44
1:B:637:ASP:CB	1:B:638:GLY:CA	2.94	0.44
1:D:636:LYS:O	1:D:639:ARG:NH1	2.47	0.44
1:A:622:ASP:O	1:A:626:ARG:HG2	2.17	0.44
1:C:544:LYS:O	1:C:547:VAL:HG22	2.18	0.44
1:D:377:GLU:O	1:D:381:GLU:OE2	2.36	0.44
1:B:552:LEU:HD23	1:B:552:LEU:HA	1.77	0.43
1:C:507:LEU:C	1:C:508:LEU:CD2	2.86	0.43
1:D:401:ILE:HD12	1:D:401:ILE:O	2.18	0.43
1:A:181:MET:HG2	1:A:254:ARG:HH22	1.84	0.43
1:A:388:PHE:O	1:A:404:GLN:HA	2.17	0.43
1:A:600:ARG:NH1	1:A:608:ASP:OD2	2.51	0.43
1:A:417:ASN:OD1	1:A:418:GLN:HG3	2.17	0.43
1:B:128:LEU:HA	1:B:131:LYS:HG3	1.99	0.43
1:D:318:GLU:O	1:D:322:ARG:HG3	2.18	0.43
1:D:639:ARG:NH1	1:D:640:GLY:H	2.17	0.43
1:A:366:LYS:HD2	1:A:366:LYS:HA	1.81	0.43
1:B:281:GLN:CB	1:B:426:ILE:HG21	2.47	0.43
1:C:423:LYS:HA	1:C:423:LYS:HD2	1.55	0.43
1:C:505:GLU:HG2	1:C:506:ILE:O	2.18	0.43
1:C:600:ARG:HG2	1:C:605:ARG:HG3	2.01	0.43
1:A:250:GLU:OE2	1:A:251:PRO:CA	2.64	0.43
1:A:506:ILE:H	1:A:506:ILE:CD1	2.31	0.43
1:B:235:TYR:HE1	1:B:261:LEU:HB3	1.83	0.43
1:C:519:ASP:HA	1:C:522:LEU:HB2	2.01	0.43
1:A:650:VAL:HG23	1:A:651:GLU:OE1	2.18	0.43
1:B:600:ARG:NH1	1:B:604:ASP:HB3	2.34	0.43
1:D:182:LEU:O	1:D:185:GLU:HB2	2.19	0.43
1:C:397:GLY:C	1:C:398:LYS:HZ2	2.22	0.43
1:A:180:ALA:O	1:A:183:LEU:HB3	2.19	0.43
1:A:225:GLN:HB2	1:A:296:LEU:HD22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:VAL:HG23	1:C:380:THR:H	1.83	0.43
1:C:463:VAL:O	1:C:530:ARG:HD3	2.19	0.43
1:B:288:LYS:NZ	3:E:10:DC:OP1	2.52	0.43
3:E:14:DA:H2"	3:E:15:DA:H8	1.83	0.43
2:N:20:DA:H2"	2:N:21:DT:C5'	2.49	0.43
1:A:127:GLU:HG2	1:A:200:ARG:HH22	1.84	0.43
1:A:469:LEU:HD22	1:A:541:PHE:CE2	2.54	0.43
1:B:190:LEU:HD22	1:B:234:ILE:HD11	2.01	0.43
1:B:588:ASN:O	1:D:641:PTR:HA	2.18	0.43
1:B:146:LEU:HA	1:B:146:LEU:HD23	1.72	0.43
1:B:392:PHE:CE1	1:B:401:ILE:HD11	2.54	0.43
4:A:751:HOH:O	1:C:646:ILE:HD13	2.16	0.43
1:D:250:GLU:HA	1:D:251:PRO:HD3	1.88	0.43
3:M:14:DA:H2"	3:M:15:DA:H8	1.84	0.43
3:M:16:DG:H2"	3:M:17:DA:C8	2.54	0.43
1:B:392:PHE:CZ	1:B:401:ILE:HD11	2.54	0.42
1:B:458:LYS:HE3	1:B:462:GLU:HG3	2.01	0.42
1:B:543:SER:O	1:B:547:VAL:HG13	2.19	0.42
4:A:751:HOH:O	1:C:646:ILE:HD11	2.16	0.42
1:D:336:SER:O	1:D:337:THR:HG22	2.18	0.42
1:A:311:VAL:HG11	1:A:358:ALA:CB	2.49	0.42
1:C:148:ARG:C	1:C:148:ARG:HD3	2.40	0.42
1:A:590:GLN:HA	1:A:591:PRO:HD3	1.93	0.42
1:B:483:ASN:HD21	1:B:508:LEU:HD23	1.85	0.42
1:C:261:LEU:O	1:C:264:VAL:HG22	2.19	0.42
1:C:399:LEU:N	1:C:400:PRO:HD3	2.34	0.42
1:C:639:ARG:N	1:C:639:ARG:HD2	2.34	0.42
1:D:133:GLY:O	1:D:137:LEU:HD12	2.19	0.42
1:B:131:LYS:O	1:B:135:ARG:HG2	2.20	0.42
1:B:225:GLN:HB2	1:B:296:LEU:HD22	2.01	0.42
1:B:398:LYS:HD3	1:B:398:LYS:HA	1.60	0.42
1:C:250:GLU:OE2	1:C:253:THR:HG21	2.20	0.42
1:D:616:TYR:HA	1:D:617:PRO:HA	1.72	0.42
1:A:222:ALA:N	1:A:223:PRO:HD2	2.34	0.42
1:A:467:ARG:CD	4:A:746:HOH:O	2.50	0.42
1:B:127:GLU:N	4:B:705:HOH:O	2.53	0.42
1:C:177:GLU:HB2	4:C:734:HOH:O	2.03	0.42
1:C:379:VAL:HG23	1:C:380:THR:N	2.34	0.42
1:A:506:ILE:H	1:A:506:ILE:HD12	1.84	0.42
1:B:579:GLY:C	1:B:580:GLN:HG2	2.39	0.42
1:C:572:THR:OG1	1:C:589:ILE:O	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:GLN:O	1:A:129:LYS:HG2	2.20	0.42
1:B:310:LEU:HD12	1:B:310:LEU:O	2.20	0.42
1:A:310:LEU:HD13	1:A:310:LEU:H	1.77	0.42
1:A:359:LEU:HG	1:A:361:LYS:HG3	2.01	0.42
1:A:378:SER:O	1:A:381:GLU:HG2	2.20	0.42
1:A:542:ILE:CG2	1:A:562:ARG:CB	2.97	0.42
1:A:547:VAL:HG11	1:A:562:ARG:HD2	2.01	0.42
1:B:639:ARG:CZ	1:B:639:ARG:HA	2.50	0.42
1:C:131:LYS:HG2	1:C:131:LYS:H	1.64	0.42
1:D:509:GLY:N	4:D:706:HOH:O	2.45	0.42
1:A:181:MET:HG2	1:A:254:ARG:HH12	1.84	0.42
1:A:281:GLN:HB3	1:A:426:ILE:HG21	2.02	0.42
1:B:503:ASN:O	1:B:513:THR:HG21	2.20	0.42
1:C:247:GLY:N	1:C:249:LEU:CD1	2.73	0.42
1:D:301:PHE:N	1:D:301:PHE:CD1	2.87	0.42
1:D:436:ASP:N	1:D:436:ASP:OD1	2.52	0.42
1:A:577:ILE:CD1	1:A:578:ARG:CB	2.98	0.42
1:C:179:LEU:C	1:C:179:LEU:HD22	2.40	0.42
1:C:394:LEU:HD22	4:C:738:HOH:O	2.11	0.42
1:D:269:VAL:HG12	1:D:297:LEU:HD12	2.02	0.42
1:B:538:ILE:HG22	1:B:540:GLY:H	1.84	0.41
1:C:295:PHE:O	1:C:356:CYS:HB3	2.21	0.41
2:F:13:DG:H2'	2:F:14:DA:C8	2.55	0.41
1:A:394:LEU:HD13	1:A:395:GLY:O	2.20	0.41
1:C:337:THR:O	1:C:337:THR:HG23	2.20	0.41
1:D:249:LEU:HD21	1:D:254:ARG:NH1	2.35	0.41
1:D:310:LEU:N	1:D:310:LEU:HD13	2.35	0.41
1:A:361:LYS:N	4:A:704:HOH:O	2.54	0.41
1:C:589:ILE:H	1:C:589:ILE:HG12	1.74	0.41
1:D:179:LEU:HA	1:D:182:LEU:HB2	2.01	0.41
1:D:311:VAL:HA	1:D:389:SER:O	2.20	0.41
1:D:484:ASP:HB3	1:D:492:PHE:CZ	2.55	0.41
2:F:13:DG:H2'	2:F:14:DA:H5"	2.02	0.41
1:A:406:LEU:HD12	1:A:406:LEU:HA	1.86	0.41
1:D:130:PHE:CZ	1:D:227:ARG:HD2	2.55	0.41
1:A:636:LYS:HB2	1:A:636:LYS:HE3	1.80	0.41
1:C:306:ALA:CB	4:C:738:HOH:O	2.68	0.41
1:C:577:ILE:N	4:C:701:HOH:O	2.53	0.41
1:D:215:ALA:HB1	1:D:216:PRO:HD2	2.03	0.41
1:A:399:LEU:CD1	1:A:401:ILE:HG23	2.51	0.41
1:A:495:ARG:NH1	1:B:534:SER:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:GLY:HA2	1:C:398:LYS:HA	1.47	0.41
1:D:342:ASN:ND2	1:D:362:ASN:OD1	2.51	0.41
1:A:394:LEU:HA	1:A:394:LEU:HD22	1.90	0.41
1:A:588:ASN:O	1:C:641:PTR:HA	2.20	0.41
1:B:339:GLU:HA	1:B:339:GLU:OE1	2.19	0.41
1:D:633:GLN:CD	1:D:633:GLN:N	2.73	0.41
1:A:360:PHE:CA	4:A:704:HOH:O	2.69	0.41
1:A:373:ARG:HD3	1:A:382:GLU:OE1	2.20	0.41
1:B:394:LEU:HD22	1:B:395:GLY:N	2.36	0.41
1:B:500:SER:O	1:B:505:GLU:N	2.52	0.41
1:C:134:LEU:HD23	1:C:135:ARG:NH1	2.36	0.41
1:C:401:ILE:HD12	1:C:401:ILE:O	2.21	0.41
1:D:183:LEU:O	1:D:186:THR:HG23	2.20	0.41
1:D:286:GLN:HA	1:D:364:LEU:HD21	2.03	0.41
2:N:19:DC:H2"	2:N:20:DA:O4'	2.21	0.41
1:A:223:PRO:O	1:A:227:ARG:HG2	2.21	0.41
1:A:393:THR:H	1:A:400:PRO:CA	2.32	0.41
1:C:633:GLN:HA	1:C:634:MET:CB	2.40	0.41
1:D:213:ASN:OD1	1:D:213:ASN:N	2.53	0.41
1:A:510:ARG:CD	1:A:510:ARG:N	2.73	0.41
1:C:232:VAL:HG11	1:C:297:LEU:HD22	2.03	0.41
1:C:240:GLN:NE2	4:C:709:HOH:O	2.53	0.41
1:D:552:LEU:HD23	1:D:552:LEU:HA	1.82	0.41
1:D:547:VAL:HG11	1:D:562:ARG:HD2	2.02	0.41
1:B:208:GLN:O	1:B:211:ALA:HB3	2.21	0.41
1:B:572:THR:OG1	1:B:589:ILE:O	2.25	0.41
1:C:144:ILE:O	1:C:148:ARG:HG3	2.21	0.41
1:A:360:PHE:C	4:A:704:HOH:O	2.59	0.40
1:B:616:TYR:HA	1:B:617:PRO:HA	1.86	0.40
1:C:210:LEU:O	1:C:212:GLY:O	2.39	0.40
1:C:367:LYS:HE2	1:C:367:LYS:HB2	1.27	0.40
1:C:617:PRO:HB2	1:C:618:LYS:HD2	2.04	0.40
3:M:17:DA:C2'	4:M:102:HOH:O	2.29	0.40
1:A:141:VAL:HA	1:A:144:ILE:CG2	2.51	0.40
1:A:439:PRO:HA	1:A:440:PHE:HA	1.60	0.40
1:B:230:SER:O	1:B:233:ASP:HB2	2.21	0.40
1:B:424:ALA:HB2	1:B:515:TRP:NE1	2.37	0.40
1:B:510:ARG:HD2	1:B:510:ARG:HH11	1.75	0.40
1:B:633:GLN:HA	1:B:633:GLN:OE1	2.20	0.40
1:C:283:LEU:HD11	1:C:289:PHE:CD1	2.56	0.40
1:C:379:VAL:HG13	3:M:6:DT:OP1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LEU:HD12	1:C:406:LEU:HA	1.81	0.40
1:A:221:LEU:HD23	1:A:294:ARG:HD3	2.02	0.40
1:A:519:ASP:HA	1:A:522:LEU:HB2	2.04	0.40
1:C:424:ALA:HB2	1:C:515:TRP:NE1	2.37	0.40
1:A:343:ASN:N	1:A:343:ASN:OD1	2.50	0.40
1:D:367:LYS:HA	1:D:367:LYS:HE2	0.60	0.40
1:D:392:PHE:CD1	1:D:401:ILE:HD11	2.57	0.40
1:D:402:GLN:H	1:D:402:GLN:CD	2.25	0.40
1:C:227:ARG:HG2	1:C:227:ARG:H	1.70	0.40
1:C:250:GLU:N	1:C:251:PRO:CD	2.84	0.40
1:C:295:PHE:HA	4:C:717:HOH:O	2.21	0.40
1:C:295:PHE:HD1	4:C:717:HOH:O	2.05	0.40
1:C:335:GLU:O	1:C:335:GLU:HG2	2.22	0.40
1:C:379:VAL:HA	4:C:732:HOH:O	2.21	0.40
2:N:13:DG:H2"	2:N:14:DA:H8	1.86	0.40
2:N:13:DG:H2"	2:N:14:DA:O5'	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	480/539 (89%)	461 (96%)	17 (4%)	2 (0%)	39	80
1	B	473/539 (88%)	455 (96%)	16 (3%)	2 (0%)	39	80
1	C	471/539 (87%)	458 (97%)	12 (2%)	1 (0%)	52	88
1	D	476/539 (88%)	462 (97%)	13 (3%)	1 (0%)	52	88
All	All	1900/2156 (88%)	1836 (97%)	58 (3%)	6 (0%)	46	85

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	637	ASP
1	A	377	GLU
1	A	396	PRO
1	B	149	GLU
1	D	216	PRO
1	C	617	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	424/459 (92%)	360 (85%)	64 (15%)	3 17
1	B	420/459 (92%)	363 (86%)	57 (14%)	5 22
1	C	420/459 (92%)	355 (84%)	65 (16%)	3 15
1	D	423/459 (92%)	351 (83%)	72 (17%)	2 12
All	All	1687/1836 (92%)	1429 (85%)	258 (15%)	3 17

All (258) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	GLU
1	A	140	ARG
1	A	143	GLU
1	A	144	ILE
1	A	147	LEU
1	A	149	GLU
1	A	179	LEU
1	A	181	MET
1	A	182	LEU
1	A	183	LEU
1	A	184	GLN
1	A	202	GLN
1	A	219	GLU
1	A	224	LEU
1	A	231	LEU
1	A	234	ILE

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Mol	Chain	Res	Type
1	A	237	GLN
1	A	249	LEU
1	A	254	ARG
1	A	256	SER
1	A	257	LEU
1	A	258	THR
1	A	288	LYS
1	A	307	LYS
1	A	310	LEU
1	A	335	GLU
1	A	337	THR
1	A	339	GLU
1	A	340	ILE
1	A	344	THR
1	A	349	ASN
1	A	351	ILE
1	A	366	LYS
1	A	370	ARG
1	A	373	ARG
1	A	374	LYS
1	A	380	THR
1	A	384	CYS
1	A	391	SER
1	A	398	LYS
1	A	401	ILE
1	A	402	GLN
1	A	435	MET
1	A	437	ARG
1	A	494	HIS
1	A	508	LEU
1	A	510	ARG
1	A	521	VAL
1	A	536	ARG
1	A	542	ILE
1	A	543	SER
1	A	578	ARG
1	A	583	SER
1	A	585	GLN
1	A	612	LEU
1	A	618	LYS
1	A	626	ARG
1	A	627	SER

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Mol	Chain	Res	Type
1	A	634	MET
1	A	636	LYS
1	A	637	ASP
1	A	639	ARG
1	A	645	THR
1	A	646	ILE
1	B	143	GLU
1	B	144	ILE
1	B	182	LEU
1	B	197	VAL
1	B	219	GLU
1	B	220	SER
1	B	221	LEU
1	B	234	ILE
1	B	236	SER
1	B	238	LEU
1	B	250	GLU
1	B	252	LYS
1	B	254	ARG
1	B	258	THR
1	B	261	LEU
1	B	282	VAL
1	B	288	LYS
1	B	307	LYS
1	B	310	LEU
1	B	312	ARG
1	B	337	THR
1	B	339	GLU
1	B	344	THR
1	B	361	LYS
1	B	366	LYS
1	B	370	ARG
1	B	380	THR
1	B	389	SER
1	B	394	LEU
1	B	398	LYS
1	B	399	LEU
1	B	402	GLN
1	B	407	SER
1	B	412	VAL
1	B	436	ASP
1	B	437	ARG

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Mol	Chain	Res	Type
1	B	449	GLU
1	B	465	THR
1	B	466	ASN
1	B	467	ARG
1	B	496	SER
1	B	500	SER
1	B	508	LEU
1	B	510	ARG
1	B	521	VAL
1	B	536	ARG
1	B	577	ILE
1	B	580	GLN
1	B	581	ASP
1	B	585	GLN
1	B	601	SER
1	B	621	LYS
1	B	632	GLU
1	B	634	MET
1	B	637	ASP
1	B	639	ARG
1	B	646	ILE
1	C	127	GLU
1	C	131	LYS
1	C	139	HIS
1	C	148	ARG
1	C	151	LEU
1	C	177	GLU
1	C	179	LEU
1	C	181	MET
1	C	182	LEU
1	C	184	GLN
1	C	196	LEU
1	C	200	ARG
1	C	202	GLN
1	C	208	GLN
1	C	213	ASN
1	C	219	GLU
1	C	236	SER
1	C	252	LYS
1	C	257	LEU
1	C	262	ASP
1	C	285	THR

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Mol	Chain	Res	Type
1	C	287	THR
1	C	297	LEU
1	C	300	ARG
1	C	307	LYS
1	C	310	LEU
1	C	312	ARG
1	C	335	GLU
1	C	336	SER
1	C	339	GLU
1	C	340	ILE
1	C	355	CYS
1	C	363	LEU
1	C	367	LYS
1	C	368	ILE
1	C	370	ARG
1	C	372	GLU
1	C	377	GLU
1	C	379	VAL
1	C	380	THR
1	C	386	VAL
1	C	394	LEU
1	C	398	LYS
1	C	402	GLN
1	C	423	LYS
1	C	435	MET
1	C	436	ASP
1	C	437	ARG
1	C	438	VAL
1	C	467	ARG
1	C	490	GLU
1	C	505	GLU
1	C	507	LEU
1	C	508	LEU
1	C	513	THR
1	C	521	VAL
1	C	531	SER
1	C	536	ARG
1	C	575	HIS
1	C	578	ARG
1	C	601	SER
1	C	618	LYS
1	C	621	LYS

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Mol	Chain	Res	Type
1	C	639	ARG
1	C	646	ILE
1	D	127	GLU
1	D	129	LYS
1	D	131	LYS
1	D	135	ARG
1	D	140	ARG
1	D	144	ILE
1	D	146	LEU
1	D	148	ARG
1	D	149	GLU
1	D	151	LEU
1	D	152	GLN
1	D	181	MET
1	D	182	LEU
1	D	185	GLU
1	D	189	GLU
1	D	196	LEU
1	D	197	VAL
1	D	202	GLN
1	D	203	ILE
1	D	213	ASN
1	D	217	PHE
1	D	237	GLN
1	D	240	GLN
1	D	249	LEU
1	D	254	ARG
1	D	256	SER
1	D	260	ARG
1	D	283	LEU
1	D	285	THR
1	D	287	THR
1	D	288	LYS
1	D	300	ARG
1	D	301	PHE
1	D	310	LEU
1	D	311	VAL
1	D	335	GLU
1	D	336	SER
1	D	341	ILE
1	D	344	THR
1	D	361	LYS

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Mol	Chain	Res	Type
1	D	367	LYS
1	D	370	ARG
1	D	371	CYS
1	D	378	SER
1	D	381	GLU
1	D	392	PHE
1	D	393	THR
1	D	394	LEU
1	D	399	LEU
1	D	402	GLN
1	D	404	GLN
1	D	414	VAL
1	D	433	SER
1	D	436	ASP
1	D	437	ARG
1	D	438	VAL
1	D	441	VAL
1	D	444	GLU
1	D	503	ASN
1	D	505	GLU
1	D	507	LEU
1	D	521	VAL
1	D	536	ARG
1	D	578	ARG
1	D	580	GLN
1	D	590	GLN
1	D	612	LEU
1	D	618	LYS
1	D	633	GLN
1	D	637	ASP
1	D	639	ARG
1	D	648	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	138	GLN
1	B	237	GLN
1	C	184	GLN
1	C	240	GLN
1	D	628	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PTR	A	641	1	13,16,17	1.17	1 (7%)	19,22,24	0.72	0
1	PTR	B	641	1	13,16,17	1.29	1 (7%)	19,22,24	0.69	0
1	PTR	C	641	1	13,16,17	1.30	1 (7%)	19,22,24	0.79	0
1	PTR	D	641	1	13,16,17	1.33	1 (7%)	19,22,24	0.70	1 (5%)

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
1	PTR	A	641	1	-	0/9/11/13	0/1/1/1
1	PTR	B	641	1	-	0/9/11/13	0/1/1/1
1	PTR	C	641	1	-	0/9/11/13	0/1/1/1
1	PTR	D	641	1	-	0/9/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	641	PTR	OH-CZ	-4.12	1.30	1.40
1	C	641	PTR	OH-CZ	-4.10	1.30	1.40
1	A	641	PTR	OH-CZ	-4.03	1.31	1.40
1	B	641	PTR	OH-CZ	-4.02	1.31	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	641	PTR	O-C-CA	-2.17	119.91	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	641	PTR	1	0
1	C	641	PTR	1	0
1	D	641	PTR	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	488/539 (90%)	-0.02	2 (0%) 93 90	56, 96, 164, 227	0
1	B	483/539 (89%)	-0.02	1 (0%) 95 94	54, 98, 164, 212	0
1	C	483/539 (89%)	-0.09	0 100 100	83, 125, 179, 217	0
1	D	486/539 (90%)	-0.09	3 (0%) 90 84	78, 122, 183, 219	0
2	F	21/21 (100%)	-0.61	0 100 100	90, 133, 214, 249	0
2	N	21/21 (100%)	-0.76	0 100 100	93, 133, 203, 228	0
3	E	21/21 (100%)	-0.74	0 100 100	111, 128, 201, 227	0
3	M	21/21 (100%)	-0.68	0 100 100	107, 124, 202, 222	0
All	All	2024/2240 (90%)	-0.08	6 (0%) 94 93	54, 114, 178, 249	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	395	GLY	3.4
1	D	586	ILE	3.0
1	A	395	GLY	2.4
1	B	336	SER	2.2
1	A	254	ARG	2.2
1	D	561	LEU	2.0

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

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	PTR	A	641	16/17	0.94	0.18	-	103,120,156,159	0
1	PTR	B	641	16/17	0.94	0.15	-	95,112,142,151	0
1	PTR	C	641	16/17	0.97	0.21	-	62,86,109,118	0
1	PTR	D	641	16/17	0.97	0.21	-	61,93,117,118	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.