



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2017 – 06:43 AM EDT

PDB ID : 2G63
Title : Crystal structure of human dipeptidyl peptidase IV (DPPIV) complexed with cyanopyrrolidine (C5-pro-pro) inhibitor 24b
Authors : Longenecker, K.L.; Fry, E.H.; Lake, M.R.; Solomon, L.R.; Pei, Z.; Li, X.
Deposited on : unknown
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

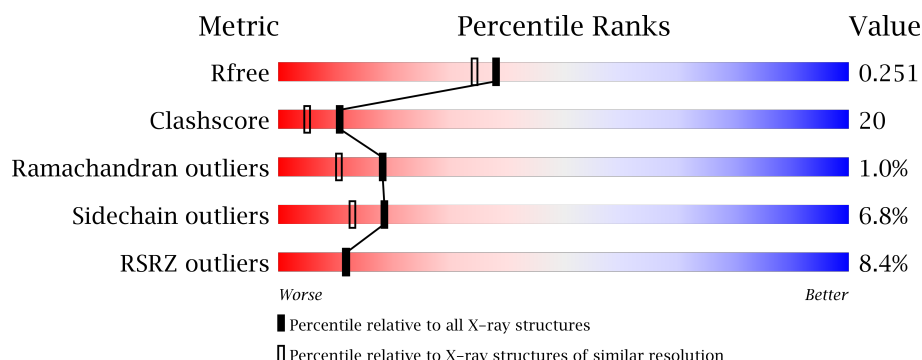
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	726	<div> <div>7%</div> <div>70% 25% .</div> </div>
1	B	726	<div> <div>9%</div> <div>69% 26% .</div> </div>
1	C	726	<div> <div>10%</div> <div>66% 30% .</div> </div>
1	D	726	<div> <div>8%</div> <div>68% 28% .</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AAF	B	800	-	-	-	X

2 Entry composition [i](#)

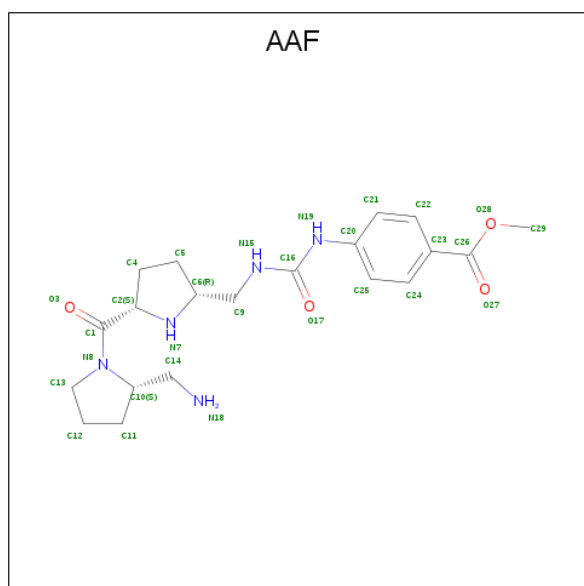
There are 3 unique types of molecules in this entry. The entry contains 28111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	B	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	C	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			
1	D	726	Total	C	N	O	S	0	0	0
			5949	3816	980	1127	26			

- Molecule 2 is METHYL 4-{[({[(2R,5S)-5-{{[(2S)-2-(AMINOMETHYL)PYRROLIDIN-1-YL] CARBONYL}PYRROLIDIN-2-YL]METHYL}AMINO)CARBONYL]AMINO}BENZOATE (three-letter code: AAF) (formula: C₂₀H₂₉N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			29	20	5	4		

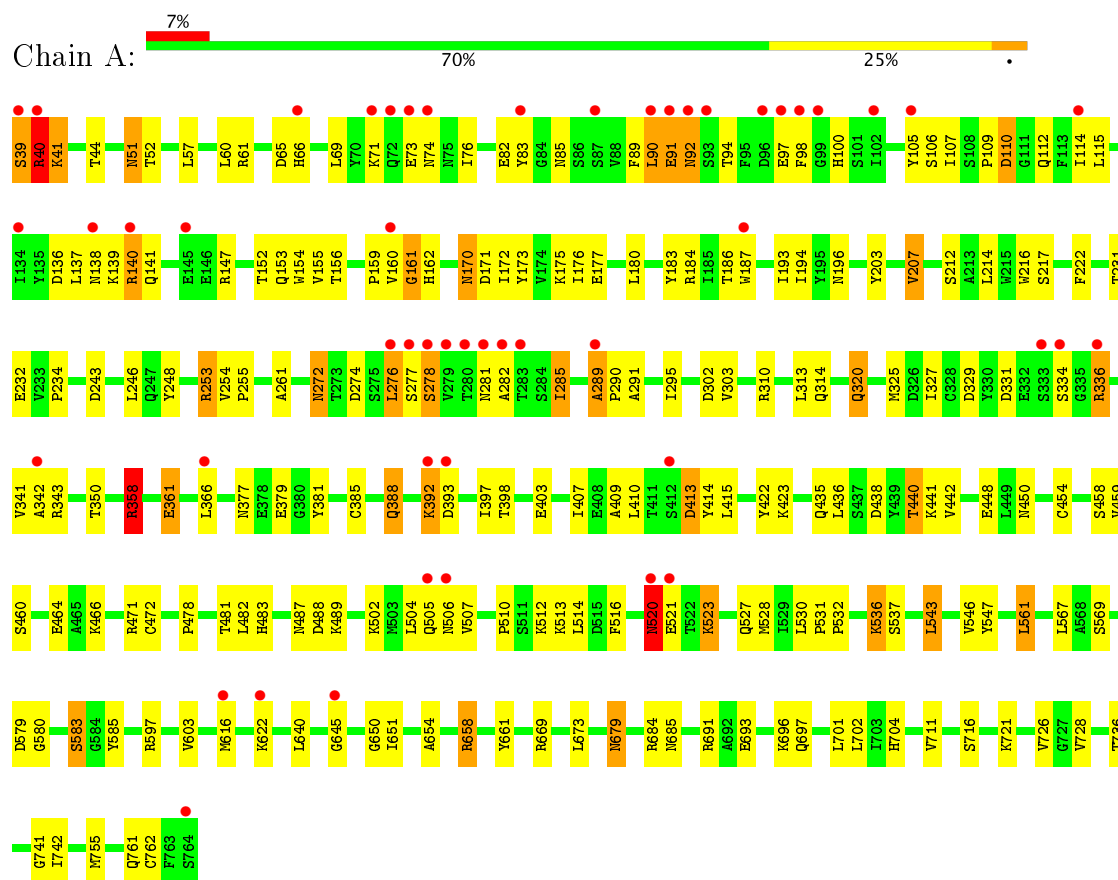
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1195	Total 1195	O 1195	0	0
3	B	1121	Total 1121	O 1121	0	0
3	C	938	Total 938	O 938	0	0
3	D	1032	Total 1032	O 1032	0	0

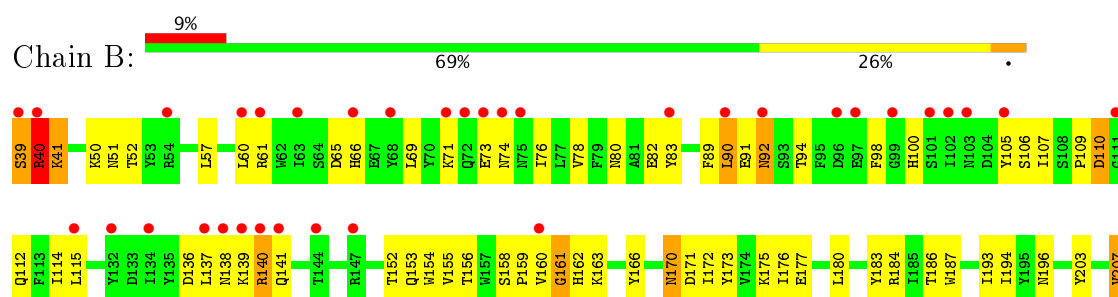
3 Residue-property plots

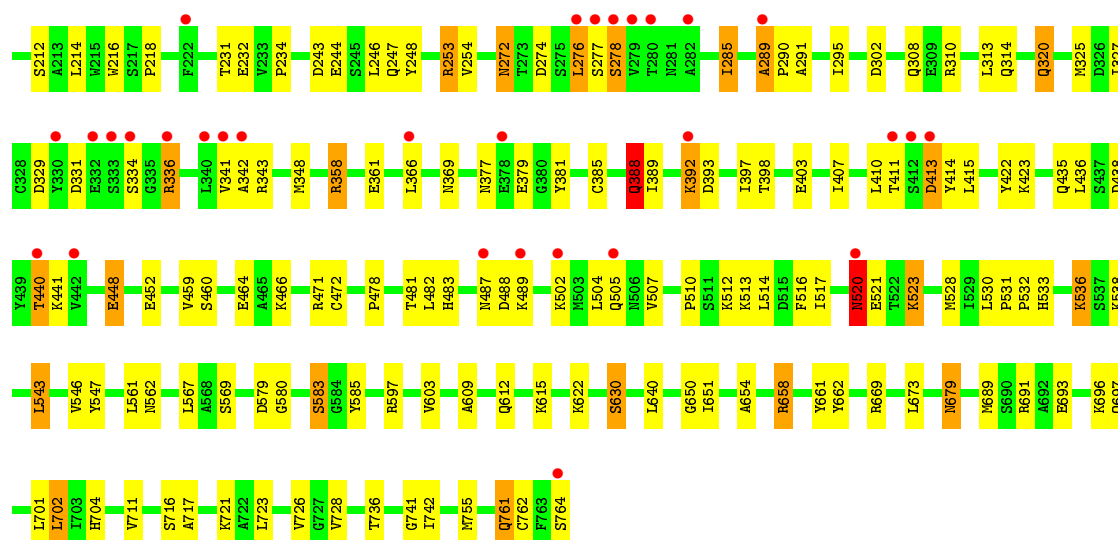
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4

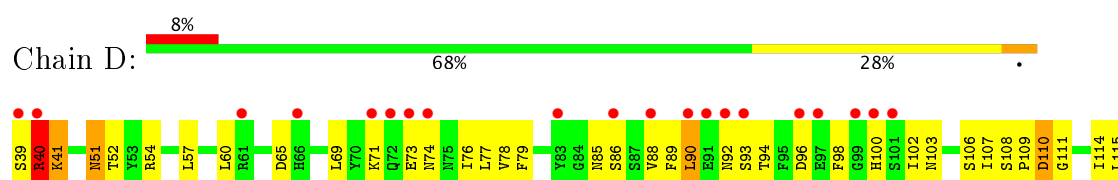


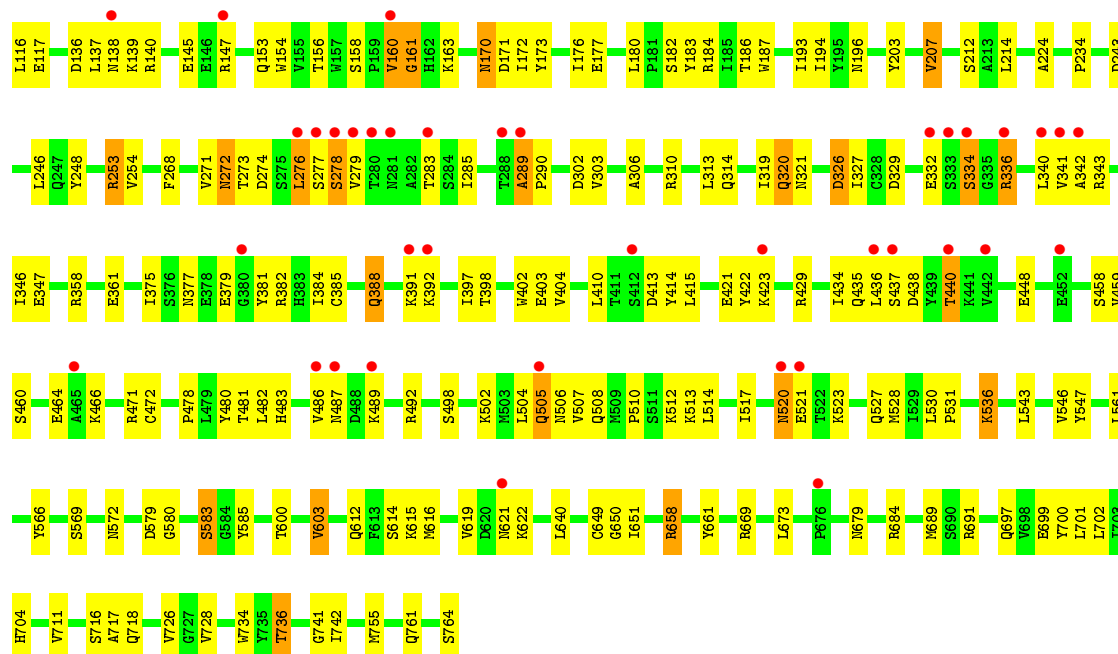


• Molecule 1: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.13Å 126.50Å 127.37Å 90.00° 96.66° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.00) 99.8 (19.96-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.251 0.214 , 0.251	Depositor DCC
R_{free} test set	12845 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 78.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28111	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/6120	0.67	4/8321 (0.0%)
1	B	0.36	1/6120 (0.0%)	0.71	4/8321 (0.0%)
1	C	0.32	0/6120	0.62	1/8321 (0.0%)
1	D	0.33	0/6120	0.62	1/8321 (0.0%)
All	All	0.34	1/24480 (0.0%)	0.66	10/33284 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	630	SER	C-O	7.92	1.38	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	358	ARG	NE-CZ-NH2	18.50	129.55	120.30
1	B	358	ARG	NE-CZ-NH1	-17.66	111.47	120.30
1	A	358	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	358	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	B	358	ARG	CD-NE-CZ	6.52	132.73	123.60
1	A	358	ARG	CD-NE-CZ	5.98	131.97	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	GLN	N-CA-C	-5.54	96.03	111.00
1	B	388	GLN	N-CA-C	-5.36	96.52	111.00
1	D	388	GLN	N-CA-C	-5.13	97.15	111.00
1	C	388	GLN	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	700	TYR	Sidechain
1	D	700	TYR	Sidechain

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	5949	0	5667	236	0
1	B	5949	0	5666	233	0
1	C	5949	0	5667	253	0
1	D	5949	0	5667	243	0
2	B	29	0	27	1	0
3	A	1195	0	0	63	0
3	B	1121	0	0	59	0
3	C	938	0	0	72	0
3	D	1032	0	0	67	0
All	All	28111	0	22694	949	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 20.

All (949) 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:A:736:THR:HB	3:B:1870:HOH:O	1.37	1.24
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.25	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ALA:HB1	1:B:290:PRO:HA	1.28	1.12
1:A:736:THR:HG21	1:B:721:LYS:HB2	1.31	1.06
1:C:114:ILE:HD11	1:C:137:LEU:HD21	1.37	1.06
1:D:114:ILE:HD11	1:D:137:LEU:HD21	1.37	1.05
1:D:289:ALA:HB1	1:D:290:PRO:HA	1.35	1.04
1:A:721:LYS:HB2	1:B:736:THR:HG21	1.35	1.02
1:C:289:ALA:HB1	1:C:290:PRO:HA	1.36	1.01
1:C:176:ILE:HD11	1:C:276:LEU:HD21	1.43	0.99
1:D:176:ILE:HD11	1:D:276:LEU:HD21	1.43	0.98
1:D:621:ASN:HB3	3:D:768:HOH:O	1.66	0.96
1:D:528:MET:HE3	1:D:530:LEU:HD21	1.49	0.95
1:C:528:MET:HE3	1:C:530:LEU:HD21	1.50	0.93
1:A:289:ALA:HB1	1:A:290:PRO:CA	1.99	0.93
1:A:736:THR:CG2	1:B:721:LYS:HB2	2.03	0.89
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.02	0.88
1:A:736:THR:HG22	3:B:802:HOH:O	1.75	0.87
1:D:40:ARG:HA	3:D:854:HOH:O	1.73	0.87
1:D:76:ILE:HD12	1:D:90:LEU:HD11	1.57	0.86
1:B:334:SER:HB3	1:B:336:ARG:NE	1.91	0.86
1:B:615:LYS:HE3	3:B:1586:HOH:O	1.76	0.86
1:D:361:GLU:HG2	3:D:933:HOH:O	1.74	0.85
1:A:310:ARG:HH12	1:A:343:ARG:NH1	1.75	0.85
1:A:334:SER:HB3	1:A:336:ARG:NE	1.92	0.85
1:D:89:PHE:HD1	1:D:90:LEU:HD12	1.42	0.85
1:C:76:ILE:HG22	3:C:1495:HOH:O	1.76	0.85
1:C:76:ILE:HD12	1:C:90:LEU:HD11	1.57	0.84
1:A:721:LYS:HB2	1:B:736:THR:CG2	2.06	0.84
1:B:160:VAL:HG23	1:B:161:GLY:H	1.43	0.84
1:A:334:SER:HB3	1:A:336:ARG:HE	1.43	0.83
1:A:487:ASN:HB2	3:A:788:HOH:O	1.77	0.83
1:A:762:CYS:HB2	3:A:1511:HOH:O	1.78	0.83
1:A:172:ILE:H	1:A:186:THR:HG22	1.43	0.83
1:B:172:ILE:H	1:B:186:THR:HG22	1.43	0.82
1:B:334:SER:HB3	1:B:336:ARG:HE	1.42	0.82
1:C:276:LEU:HD22	1:C:276:LEU:H	1.45	0.82
1:A:289:ALA:HB2	3:A:1489:HOH:O	1.80	0.81
1:D:276:LEU:HD22	1:D:276:LEU:H	1.43	0.81
1:A:253:ARG:HH22	1:B:253:ARG:HH22	1.25	0.81
1:B:310:ARG:HH12	1:B:343:ARG:NH1	1.79	0.81
1:B:702:LEU:HD22	3:B:1886:HOH:O	1.80	0.81
1:C:89:PHE:HD1	1:C:90:LEU:HD12	1.42	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ILE:H	1:C:186:THR:HG22	1.46	0.80
1:C:528:MET:CE	1:C:530:LEU:HD21	2.12	0.80
1:B:140:ARG:HG2	1:B:140:ARG:HH11	1.48	0.79
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.48	0.79
1:A:160:VAL:HG23	1:A:161:GLY:H	1.45	0.79
1:D:172:ILE:H	1:D:186:THR:HG22	1.46	0.79
1:B:276:LEU:HB3	3:B:1234:HOH:O	1.82	0.79
1:A:341:VAL:O	1:A:342:ALA:HB3	1.82	0.79
1:D:528:MET:CE	1:D:530:LEU:HD21	2.13	0.78
1:B:207:VAL:O	1:B:358:ARG:NH2	2.16	0.78
1:A:358:ARG:NH1	3:A:1447:HOH:O	2.17	0.78
1:A:281:ASN:HB2	3:A:1179:HOH:O	1.84	0.78
1:B:448:GLU:HG3	3:B:1613:HOH:O	1.84	0.78
1:D:726:VAL:HG12	1:D:728:VAL:HG23	1.66	0.77
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.67	0.77
1:C:334:SER:HB3	1:C:336:ARG:HE	1.48	0.77
1:D:334:SER:HB3	1:D:336:ARG:HE	1.48	0.77
1:B:176:ILE:HD11	1:B:276:LEU:HD21	1.66	0.77
1:C:726:VAL:HG12	1:C:728:VAL:HG23	1.66	0.77
1:A:255:PRO:HD2	3:A:1931:HOH:O	1.83	0.77
1:A:289:ALA:CB	1:A:290:PRO:HA	2.12	0.76
1:A:282:ALA:HB3	3:A:1913:HOH:O	1.84	0.76
1:A:489:LYS:HB3	1:A:489:LYS:NZ	2.01	0.76
1:B:528:MET:HE3	1:B:530:LEU:HD21	1.68	0.76
1:A:176:ILE:HD11	1:A:276:LEU:HD21	1.67	0.76
1:B:341:VAL:HB	3:B:887:HOH:O	1.86	0.75
1:C:717:ALA:O	1:D:736:THR:HG21	1.86	0.75
1:A:505:GLN:HB3	3:A:1559:HOH:O	1.85	0.75
1:A:52:THR:HG22	3:A:1873:HOH:O	1.85	0.75
1:D:289:ALA:HB1	1:D:290:PRO:CA	2.15	0.75
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.69	0.75
1:B:489:LYS:NZ	1:B:489:LYS:HB3	2.00	0.75
1:B:517:ILE:HD13	3:B:1143:HOH:O	1.87	0.75
1:B:289:ALA:CB	1:B:290:PRO:HA	2.15	0.74
1:B:723:LEU:HA	3:B:1900:HOH:O	1.86	0.74
1:A:438:ASP:OD1	1:A:440:THR:HB	1.87	0.74
1:C:90:LEU:O	1:C:90:LEU:HD22	1.86	0.74
1:C:736:THR:HG21	1:D:717:ALA:O	1.88	0.74
1:C:289:ALA:HB1	1:C:290:PRO:CA	2.16	0.74
1:D:90:LEU:O	1:D:90:LEU:HD22	1.87	0.74
1:B:528:MET:CE	1:B:530:LEU:HD21	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:TYR:HE1	1:C:277:SER:O	1.71	0.74
1:B:184:ARG:HD3	1:B:186:THR:O	1.88	0.74
1:B:327:ILE:HB	1:B:343:ARG:HG2	1.69	0.74
1:C:276:LEU:HB3	3:C:1068:HOH:O	1.88	0.73
1:D:614:SER:HB2	3:D:768:HOH:O	1.88	0.73
1:D:289:ALA:HB2	3:D:1585:HOH:O	1.88	0.73
1:A:171:ASP:OD1	1:A:186:THR:HG23	1.88	0.73
1:C:272:ASN:ND2	1:C:274:ASP:H	1.86	0.73
1:A:350:THR:HG23	3:A:1787:HOH:O	1.89	0.73
1:D:272:ASN:ND2	1:D:274:ASP:H	1.87	0.73
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.70	0.73
1:C:594:ILE:HG13	3:C:1263:HOH:O	1.89	0.72
1:A:622:LYS:HE3	3:A:1560:HOH:O	1.88	0.72
1:B:171:ASP:OD1	1:B:186:THR:HG23	1.90	0.72
1:A:528:MET:CE	1:A:530:LEU:HD21	2.19	0.72
1:A:184:ARG:HD3	1:A:186:THR:O	1.89	0.72
1:C:684:ARG:HD3	3:C:1582:HOH:O	1.89	0.72
1:A:207:VAL:O	1:A:358:ARG:NH2	2.23	0.71
1:D:320:GLN:OE1	1:D:669:ARG:HD3	1.91	0.71
1:D:684:ARG:HG3	3:D:1162:HOH:O	1.89	0.71
1:C:361:GLU:HG2	3:C:955:HOH:O	1.89	0.71
1:B:438:ASP:OD1	1:B:440:THR:HB	1.90	0.71
1:D:183:TYR:HE1	1:D:277:SER:O	1.73	0.71
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.26	0.70
1:D:673:LEU:HG	3:D:1710:HOH:O	1.89	0.70
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.26	0.70
1:C:142:LEU:HG	3:C:1702:HOH:O	1.89	0.70
1:D:334:SER:HB3	1:D:336:ARG:NE	2.07	0.70
1:C:177:GLU:HB2	1:C:180:LEU:HD22	1.72	0.70
1:C:334:SER:HB3	1:C:336:ARG:NE	2.07	0.70
1:B:341:VAL:O	1:B:342:ALA:HB3	1.90	0.70
1:A:597:ARG:HH12	1:A:679:ASN:HD21	1.40	0.70
1:D:177:GLU:HB2	1:D:180:LEU:HD22	1.72	0.70
1:C:359:PRO:HA	3:C:1500:HOH:O	1.92	0.70
1:C:320:GLN:OE1	1:C:669:ARG:HD3	1.92	0.70
1:D:600:THR:O	1:D:603:VAL:HG13	1.92	0.70
1:C:153:GLN:HE22	1:C:170:ASN:ND2	1.90	0.69
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.74	0.69
1:D:379:GLU:HB2	3:D:1305:HOH:O	1.91	0.69
1:B:597:ARG:HH12	1:B:679:ASN:HD21	1.40	0.69
1:B:704:HIS:HB2	3:B:1886:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HD3	1:D:186:THR:O	1.92	0.69
1:D:153:GLN:HE22	1:D:170:ASN:ND2	1.90	0.69
1:A:392:LYS:HG3	3:A:1107:HOH:O	1.91	0.69
1:B:471:ARG:HB3	3:B:1550:HOH:O	1.92	0.69
1:A:327:ILE:HB	1:A:343:ARG:HG2	1.75	0.68
1:C:103:ASN:HB2	3:C:1205:HOH:O	1.92	0.68
1:C:600:THR:O	1:C:603:VAL:HG13	1.93	0.68
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.94	0.68
1:D:347:GLU:HG3	3:D:1766:HOH:O	1.94	0.68
1:A:51:ASN:HB2	3:A:972:HOH:O	1.93	0.68
1:A:97:GLU:HB3	3:A:1936:HOH:O	1.93	0.68
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.76	0.68
3:A:771:HOH:O	1:B:736:THR:HG22	1.92	0.68
1:C:184:ARG:HD3	1:C:186:THR:O	1.94	0.68
1:C:358:ARG:HD2	3:C:1669:HOH:O	1.93	0.68
1:A:253:ARG:HD3	3:A:1922:HOH:O	1.93	0.67
1:A:90:LEU:O	1:A:90:LEU:HD13	1.94	0.67
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.94	0.67
1:C:109:PRO:HB2	1:C:160:VAL:O	1.94	0.67
1:D:109:PRO:HB2	1:D:160:VAL:O	1.93	0.67
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.75	0.67
1:A:450:ASN:HB3	3:A:1607:HOH:O	1.94	0.67
1:B:90:LEU:O	1:B:90:LEU:HD13	1.95	0.67
1:C:98:PHE:HA	3:C:1652:HOH:O	1.93	0.67
1:A:310:ARG:NE	3:A:1515:HOH:O	2.26	0.67
1:A:74:ASN:C	1:A:92:ASN:HB3	2.15	0.67
1:B:74:ASN:C	1:B:92:ASN:HB3	2.15	0.67
1:C:203:TYR:HA	1:C:207:VAL:CG1	2.25	0.67
1:C:82:GLU:HG2	3:C:1535:HOH:O	1.94	0.66
1:D:203:TYR:CD2	1:D:207:VAL:HG11	2.29	0.66
1:D:203:TYR:HA	1:D:207:VAL:CG1	2.25	0.66
1:D:69:LEU:CD1	1:D:107:ILE:HD12	2.25	0.66
1:C:203:TYR:CD2	1:C:207:VAL:HG11	2.30	0.66
1:C:69:LEU:CD1	1:C:107:ILE:HD12	2.25	0.66
1:B:272:ASN:ND2	1:B:274:ASP:H	1.94	0.66
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.78	0.66
1:B:379:GLU:HB2	3:B:1743:HOH:O	1.94	0.66
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.78	0.66
1:D:171:ASP:OD1	1:D:186:THR:HG23	1.96	0.66
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.78	0.66
1:B:52:THR:HB	3:B:1656:HOH:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LYS:HG2	3:C:1268:HOH:O	1.95	0.65
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.77	0.65
1:B:109:PRO:HB2	1:B:160:VAL:O	1.96	0.65
1:D:276:LEU:H	1:D:276:LEU:CD2	2.10	0.65
1:A:272:ASN:ND2	1:A:274:ASP:H	1.95	0.65
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.95	0.65
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.78	0.64
1:D:580:GLY:O	1:D:583:SER:HB2	1.97	0.64
1:C:171:ASP:OD1	1:C:186:THR:HG23	1.97	0.64
1:C:489:LYS:HB3	1:C:489:LYS:NZ	2.13	0.64
1:D:489:LYS:HB3	1:D:489:LYS:NZ	2.12	0.64
1:A:160:VAL:HG23	1:A:161:GLY:N	2.13	0.64
1:C:361:GLU:HG2	3:C:1108:HOH:O	1.97	0.64
1:D:279:VAL:HB	3:D:1273:HOH:O	1.97	0.64
1:B:65:ASP:OD2	1:B:466:LYS:HB2	1.98	0.64
1:D:40:ARG:HH11	1:D:40:ARG:HG2	1.63	0.64
1:A:41:LYS:HB2	3:A:1293:HOH:O	1.98	0.64
1:A:697:GLN:HG3	3:A:1278:HOH:O	1.97	0.64
1:C:51:ASN:HB2	3:C:1687:HOH:O	1.98	0.63
1:A:109:PRO:HB2	1:A:160:VAL:O	1.99	0.63
1:A:276:LEU:H	1:A:276:LEU:CD2	2.12	0.63
1:B:762:CYS:HB2	3:B:1418:HOH:O	1.98	0.63
1:C:319:ILE:HG13	3:C:1697:HOH:O	1.98	0.63
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.96	0.63
1:A:65:ASP:OD2	1:A:466:LYS:HB2	1.99	0.63
1:A:693:GLU:OE1	1:A:696:LYS:HE2	1.97	0.63
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.34	0.63
1:B:693:GLU:OE1	1:B:696:LYS:HE2	1.98	0.63
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.34	0.63
1:B:160:VAL:HG23	1:B:161:GLY:N	2.12	0.63
1:B:276:LEU:CD2	1:B:276:LEU:H	2.12	0.63
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.33	0.62
1:A:726:VAL:HG12	1:A:728:VAL:HG23	1.81	0.62
1:C:580:GLY:O	1:C:583:SER:HB2	1.99	0.62
1:C:684:ARG:HD2	3:C:1685:HOH:O	2.00	0.62
1:D:71:LYS:HB3	3:D:1461:HOH:O	1.98	0.62
1:B:243:ASP:HB3	3:B:1378:HOH:O	1.99	0.62
1:B:272:ASN:HD22	1:B:274:ASP:H	1.46	0.62
1:D:341:VAL:O	1:D:342:ALA:HB3	2.00	0.62
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.30	0.62
1:C:272:ASN:HD22	1:C:274:ASP:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:PRO:HG3	1:C:326:ASP:OD2	2.00	0.62
1:D:486:VAL:HG13	1:D:487:ASN:N	2.15	0.61
1:D:54:ARG:HG2	3:D:1295:HOH:O	2.01	0.61
1:D:346:ILE:HG13	3:D:1329:HOH:O	1.99	0.61
1:C:40:ARG:HG2	1:C:40:ARG:HH11	1.65	0.61
1:D:410:LEU:HD13	1:D:415:LEU:HD23	1.82	0.61
1:B:483:HIS:HD2	3:B:921:HOH:O	1.83	0.61
1:C:390:ASP:HB3	3:C:857:HOH:O	1.99	0.61
1:D:52:THR:HG21	3:D:1570:HOH:O	1.99	0.61
1:C:114:ILE:CD1	1:C:137:LEU:HD21	2.24	0.61
1:C:486:VAL:HG13	1:C:487:ASN:N	2.16	0.61
1:B:277:SER:O	1:B:278:SER:HB3	2.00	0.61
1:C:341:VAL:O	1:C:342:ALA:HB3	2.01	0.61
1:A:277:SER:O	1:A:278:SER:HB3	2.00	0.61
1:A:272:ASN:HD22	1:A:274:ASP:H	1.49	0.60
1:B:74:ASN:HB3	1:B:92:ASN:CB	2.31	0.60
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.83	0.60
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.83	0.60
1:C:410:LEU:HD13	1:C:415:LEU:HD23	1.83	0.60
1:C:76:ILE:HB	1:C:90:LEU:CD1	2.30	0.60
1:D:114:ILE:CD1	1:D:137:LEU:HD21	2.23	0.60
1:B:489:LYS:HB3	1:B:489:LYS:HZ3	1.66	0.60
1:A:366:LEU:HD23	3:A:1245:HOH:O	2.00	0.60
1:C:276:LEU:H	1:C:276:LEU:CD2	2.11	0.60
1:C:77:LEU:HD23	1:C:88:VAL:HA	1.84	0.60
1:D:77:LEU:HD23	1:D:88:VAL:HA	1.84	0.60
1:A:377:ASN:HB2	1:A:381:TYR:O	2.02	0.60
1:C:614:SER:HA	1:C:619:VAL:HB	1.84	0.60
1:D:614:SER:HA	1:D:619:VAL:HB	1.83	0.60
1:C:272:ASN:C	1:C:272:ASN:HD22	2.05	0.60
1:D:290:PRO:HG3	1:D:326:ASP:OD2	2.01	0.60
1:D:76:ILE:HB	1:D:90:LEU:CD1	2.31	0.60
1:B:471:ARG:HD2	3:B:1711:HOH:O	2.02	0.60
1:D:140:ARG:HH11	1:D:140:ARG:HG2	1.66	0.60
1:D:272:ASN:HD22	1:D:272:ASN:C	2.05	0.60
1:C:193:ILE:HG22	1:C:194:ILE:HG13	1.84	0.60
1:C:140:ARG:HG2	1:C:140:ARG:HH11	1.67	0.59
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.83	0.59
1:C:65:ASP:OD2	1:C:466:LYS:HB2	2.02	0.59
1:D:182:SER:HB3	3:D:1765:HOH:O	2.03	0.59
1:A:261:ALA:HB2	3:B:1915:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LYS:HD3	3:B:1081:HOH:O	2.01	0.59
1:D:336:ARG:HB3	3:D:1546:HOH:O	2.03	0.59
1:D:93:SER:HB2	1:D:96:ASP:OD2	2.02	0.59
1:B:691:ARG:NE	3:B:1749:HOH:O	2.18	0.59
1:B:114:ILE:CD1	1:B:137:LEU:HD21	2.32	0.59
1:B:612:GLN:HB2	3:B:1143:HOH:O	2.03	0.59
1:A:114:ILE:CD1	1:A:137:LEU:HD21	2.31	0.59
1:B:289:ALA:HB2	3:B:1085:HOH:O	2.02	0.59
1:B:377:ASN:HB2	1:B:381:TYR:O	2.02	0.59
1:B:693:GLU:HA	1:B:726:VAL:HG11	1.85	0.59
1:C:721:LYS:HG2	3:C:1313:HOH:O	2.01	0.59
1:C:651:ILE:HG21	1:C:755:MET:HE2	1.85	0.59
1:C:93:SER:HB2	1:C:96:ASP:OD2	2.02	0.59
1:C:513:LYS:HD2	3:C:1508:HOH:O	2.03	0.59
1:D:65:ASP:OD2	1:D:466:LYS:HB2	2.02	0.59
1:A:139:LYS:HD3	3:A:1411:HOH:O	2.02	0.58
1:D:342:ALA:HA	3:D:1699:HOH:O	2.02	0.58
1:A:89:PHE:CE1	1:A:107:ILE:HD13	2.38	0.58
1:C:184:ARG:HD2	1:C:187:TRP:CE2	2.38	0.58
1:A:71:LYS:HG2	1:A:76:ILE:HG12	1.85	0.58
1:B:348:MET:HG3	3:B:1665:HOH:O	2.03	0.58
1:C:194:ILE:HD12	3:C:1007:HOH:O	2.02	0.58
1:C:338:ASN:HB2	3:C:1328:HOH:O	2.03	0.58
1:A:334:SER:CB	1:A:336:ARG:HE	2.15	0.58
1:A:651:ILE:HG21	1:A:755:MET:CE	2.34	0.58
1:D:272:ASN:HD22	1:D:274:ASP:H	1.48	0.58
1:A:506:ASN:HB2	3:A:1502:HOH:O	2.03	0.58
1:B:172:ILE:H	1:B:186:THR:CG2	2.13	0.58
1:B:248:TYR:HE1	3:B:1915:HOH:O	1.85	0.58
1:C:103:ASN:OD1	1:C:117:GLU:HG2	2.03	0.58
1:D:194:ILE:HD12	3:D:1007:HOH:O	2.03	0.58
1:D:193:ILE:HG22	1:D:194:ILE:HG13	1.85	0.58
1:B:523:LYS:HG2	3:B:1411:HOH:O	2.04	0.58
1:C:172:ILE:HB	3:C:1474:HOH:O	2.03	0.58
1:D:41:LYS:HD2	3:D:1713:HOH:O	2.02	0.58
1:A:341:VAL:O	1:A:342:ALA:CB	2.47	0.58
1:B:71:LYS:HG2	1:B:76:ILE:HG12	1.86	0.58
1:B:334:SER:CB	1:B:336:ARG:HE	2.14	0.58
1:B:452:GLU:HG2	3:B:1827:HOH:O	2.03	0.58
1:D:184:ARG:HD2	1:D:187:TRP:CE2	2.39	0.58
1:D:327:ILE:HB	1:D:343:ARG:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ASN:HB3	1:B:92:ASN:HB3	1.86	0.57
1:C:422:TYR:CE2	1:C:423:LYS:HD3	2.39	0.57
1:D:621:ASN:HB3	3:D:1531:HOH:O	2.03	0.57
1:B:651:ILE:HG21	1:B:755:MET:CE	2.34	0.57
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.40	0.57
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.86	0.57
1:C:203:TYR:HA	1:C:207:VAL:HG12	1.86	0.57
1:A:172:ILE:H	1:A:186:THR:CG2	2.15	0.57
1:D:41:LYS:HB2	3:D:1768:HOH:O	2.04	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.57
1:D:651:ILE:CD1	1:D:755:MET:HE2	2.34	0.57
1:A:684:ARG:HD2	3:A:1478:HOH:O	2.05	0.57
1:C:106:SER:HB3	1:C:115:LEU:HB3	1.85	0.57
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.85	0.57
1:A:243:ASP:HB3	3:A:1428:HOH:O	2.05	0.57
1:A:44:THR:HB	3:A:1011:HOH:O	2.04	0.57
1:B:232:GLU:HG2	3:B:1795:HOH:O	2.05	0.57
1:A:489:LYS:HB3	1:A:489:LYS:HZ3	1.70	0.56
1:A:74:ASN:HB3	1:A:92:ASN:HB3	1.85	0.56
1:D:103:ASN:OD1	1:D:117:GLU:HG2	2.04	0.56
1:A:71:LYS:HB3	3:A:1376:HOH:O	2.05	0.56
1:C:156:THR:HG21	1:C:214:LEU:HD11	1.87	0.56
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.87	0.56
1:B:651:ILE:CD1	1:B:755:MET:HE2	2.35	0.56
1:C:704:HIS:HD2	1:C:716:SER:OG	1.88	0.56
1:D:651:ILE:HG21	1:D:755:MET:CE	2.34	0.56
1:A:651:ILE:HD13	1:A:755:MET:HE2	1.87	0.56
1:C:69:LEU:HD22	3:C:1495:HOH:O	2.03	0.56
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.87	0.56
1:C:327:ILE:HB	1:C:343:ARG:HG2	1.86	0.56
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.85	0.56
1:D:277:SER:O	1:D:278:SER:HB3	2.05	0.56
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.25	0.56
1:C:651:ILE:HG21	1:C:755:MET:CE	2.36	0.56
1:B:538:LYS:HG2	3:B:1442:HOH:O	2.06	0.56
1:D:512:LYS:HD3	3:D:1446:HOH:O	2.06	0.56
1:D:622:LYS:HE3	3:D:1439:HOH:O	2.06	0.56
1:A:272:ASN:C	1:A:272:ASN:HD22	2.10	0.56
1:D:203:TYR:HA	1:D:207:VAL:HG12	1.87	0.56
1:D:156:THR:HG21	1:D:214:LEU:HD11	1.87	0.55
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.26	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:TYR:CE1	1:C:277:SER:O	2.58	0.55
1:C:40:ARG:HD2	1:C:508:GLN:HG3	1.88	0.55
1:C:69:LEU:HD13	1:C:107:ILE:HD12	1.88	0.55
1:C:71:LYS:HE2	3:C:1293:HOH:O	2.06	0.55
1:A:276:LEU:HB3	3:A:1157:HOH:O	2.06	0.55
1:B:487:ASN:HB2	3:B:1750:HOH:O	2.05	0.55
1:D:69:LEU:HD13	1:D:107:ILE:HD12	1.88	0.55
1:A:407:ILE:HG23	1:A:415:LEU:HD21	1.89	0.55
1:A:651:ILE:CD1	1:A:755:MET:HE2	2.37	0.55
1:C:340:LEU:O	1:C:343:ARG:HB3	2.07	0.55
1:D:183:TYR:CD2	1:D:276:LEU:HG	2.41	0.55
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.41	0.55
1:D:278:SER:HA	3:D:1433:HOH:O	2.06	0.55
1:D:342:ALA:HB1	3:D:1637:HOH:O	2.07	0.55
1:A:170:ASN:N	1:A:170:ASN:HD22	2.04	0.55
1:A:435:GLN:NE2	1:A:441:LYS:CD	2.70	0.55
1:C:277:SER:O	1:C:278:SER:HB3	2.06	0.55
1:A:413:ASP:HB2	3:A:1527:HOH:O	2.05	0.55
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.90	0.55
1:D:651:ILE:HD13	1:D:755:MET:HE2	1.88	0.54
1:B:413:ASP:HB2	3:B:1889:HOH:O	2.07	0.54
1:D:379:GLU:HG2	3:D:1512:HOH:O	2.06	0.54
1:D:726:VAL:CG1	1:D:728:VAL:HG23	2.37	0.54
1:D:40:ARG:HD2	1:D:508:GLN:HG3	1.88	0.54
1:D:71:LYS:HE2	3:D:1440:HOH:O	2.06	0.54
1:A:281:ASN:ND2	3:A:1642:HOH:O	2.39	0.54
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.89	0.54
1:B:114:ILE:HD12	1:B:137:LEU:HD21	1.89	0.54
1:B:651:ILE:HD13	1:B:755:MET:HE2	1.88	0.54
1:C:183:TYR:CD2	1:C:276:LEU:HG	2.41	0.54
1:C:579:ASP:HB3	1:C:583:SER:OG	2.07	0.54
1:D:170:ASN:N	1:D:170:ASN:HD22	2.06	0.54
1:A:184:ARG:HD2	1:A:187:TRP:CD2	2.42	0.54
1:B:170:ASN:N	1:B:170:ASN:HD22	2.06	0.54
1:D:651:ILE:HG21	1:D:755:MET:HE2	1.89	0.54
1:A:658:ARG:NH2	1:B:244:GLU:OE2	2.40	0.54
1:B:272:ASN:C	1:B:272:ASN:HD22	2.10	0.54
1:B:183:TYR:HE1	1:B:277:SER:O	1.91	0.54
1:B:704:HIS:HD2	1:B:716:SER:OG	1.91	0.54
1:C:57:LEU:HD21	3:C:1553:HOH:O	2.08	0.54
1:A:459:VAL:HG22	1:A:460:SER:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ALA:CB	1:B:290:PRO:CA	2.78	0.54
1:C:651:ILE:CD1	1:C:755:MET:HE2	2.38	0.54
1:D:340:LEU:O	1:D:343:ARG:HB3	2.07	0.54
1:A:597:ARG:NH1	1:A:679:ASN:HD21	2.06	0.54
1:C:332:GLU:HB2	3:C:1548:HOH:O	2.07	0.54
1:D:289:ALA:CB	1:D:290:PRO:HA	2.24	0.53
1:D:615:LYS:NZ	3:D:1056:HOH:O	2.41	0.53
1:B:502:LYS:O	1:B:505:GLN:HG2	2.09	0.53
1:D:704:HIS:HD2	1:D:716:SER:OG	1.91	0.53
1:A:114:ILE:HD12	1:A:137:LEU:HD21	1.89	0.53
1:C:341:VAL:HG12	3:C:1320:HOH:O	2.07	0.53
1:A:379:GLU:HG3	3:A:1198:HOH:O	2.07	0.53
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.44	0.53
1:B:726:VAL:HB	3:B:1900:HOH:O	2.08	0.53
1:A:704:HIS:HD2	1:A:716:SER:OG	1.92	0.53
1:C:486:VAL:HG13	1:C:487:ASN:H	1.73	0.53
1:D:147:ARG:HB2	3:D:1010:HOH:O	2.09	0.53
1:C:243:ASP:HB3	3:C:1034:HOH:O	2.09	0.53
1:D:615:LYS:HG2	3:D:1056:HOH:O	2.08	0.53
1:B:90:LEU:HD22	1:B:90:LEU:C	2.28	0.53
1:A:658:ARG:O	1:A:658:ARG:HG3	2.08	0.53
1:B:389:ILE:HD13	3:B:1167:HOH:O	2.08	0.53
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.89	0.53
1:B:520:ASN:O	1:B:521:GLU:HB2	2.09	0.53
1:C:333:SER:HB2	3:C:1523:HOH:O	2.09	0.53
1:C:651:ILE:HD13	1:C:755:MET:HE2	1.91	0.53
1:B:407:ILE:HG23	1:B:415:LEU:HD21	1.91	0.52
1:A:90:LEU:HD22	1:A:90:LEU:C	2.30	0.52
1:C:342:ALA:HB3	3:C:1701:HOH:O	2.08	0.52
1:D:579:ASP:HB3	1:D:583:SER:OG	2.10	0.52
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.90	0.52
1:A:520:ASN:O	1:A:521:GLU:HB2	2.09	0.52
1:C:105:TYR:HB2	3:C:1293:HOH:O	2.09	0.52
1:D:486:VAL:HG13	1:D:487:ASN:H	1.73	0.52
1:A:622:LYS:NZ	1:A:622:LYS:HB2	2.25	0.52
1:A:736:THR:HG21	1:B:721:LYS:CB	2.22	0.52
1:C:736:THR:HG23	3:D:778:HOH:O	2.10	0.52
1:D:377:ASN:HB3	1:D:379:GLU:H	1.73	0.52
1:D:40:ARG:NH1	3:D:1185:HOH:O	2.42	0.52
1:A:502:LYS:O	1:A:505:GLN:HG2	2.09	0.52
1:B:471:ARG:HG3	3:B:1697:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:HD3	1:C:507:VAL:C	2.30	0.52
1:A:183:TYR:HE1	1:A:277:SER:O	1.92	0.52
1:B:69:LEU:HD13	1:B:107:ILE:HD12	1.91	0.52
1:A:325:MET:HE2	1:A:327:ILE:HG12	1.92	0.52
1:C:89:PHE:CE1	1:C:107:ILE:HD13	2.45	0.52
1:D:76:ILE:HB	1:D:90:LEU:HD13	1.91	0.52
1:A:435:GLN:NE2	1:A:441:LYS:HD2	2.25	0.52
1:B:140:ARG:NH1	1:B:140:ARG:HG2	2.21	0.52
1:A:276:LEU:N	1:A:276:LEU:CD2	2.73	0.52
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.92	0.52
1:C:422:TYR:CD2	1:C:423:LYS:HD3	2.45	0.52
1:D:422:TYR:CE2	1:D:423:LYS:HD3	2.44	0.52
1:D:40:ARG:HD3	1:D:507:VAL:C	2.30	0.52
1:A:342:ALA:HB3	3:A:1804:HOH:O	2.08	0.51
1:A:379:GLU:HG2	1:A:381:TYR:CD1	2.45	0.51
1:D:536:LYS:HE2	3:D:1692:HOH:O	2.10	0.51
1:D:658:ARG:HG2	1:D:661:TYR:CE2	2.45	0.51
1:C:726:VAL:CG1	1:C:728:VAL:HG23	2.38	0.51
1:C:76:ILE:HB	1:C:90:LEU:HD13	1.91	0.51
1:C:99:GLY:HA3	3:C:1653:HOH:O	2.10	0.51
1:D:94:THR:HB	3:D:1445:HOH:O	2.09	0.51
1:A:397:ILE:HG13	1:A:398:THR:HG23	1.92	0.51
1:D:472:CYS:O	1:D:478:PRO:HA	2.10	0.51
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.45	0.51
1:C:170:ASN:HD22	1:C:170:ASN:N	2.08	0.51
1:C:377:ASN:HB2	1:C:381:TYR:O	2.11	0.51
1:B:597:ARG:NH1	1:B:679:ASN:HD21	2.06	0.51
1:C:536:LYS:HE3	3:C:1111:HOH:O	2.11	0.51
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.91	0.51
1:D:183:TYR:CE1	1:D:277:SER:O	2.60	0.51
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.21	0.51
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.46	0.51
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.75	0.51
1:C:377:ASN:HB3	1:C:379:GLU:H	1.75	0.51
1:D:89:PHE:CE1	1:D:107:ILE:HD13	2.46	0.51
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.93	0.51
1:B:513:LYS:HE3	1:B:530:LEU:HD11	1.93	0.51
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.32	0.51
1:D:277:SER:HA	3:D:1719:HOH:O	2.10	0.51
1:A:285:ILE:N	1:A:285:ILE:CD1	2.74	0.50
1:B:516:PHE:CE2	1:B:523:LYS:HE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:SER:O	1:C:40:ARG:O	2.29	0.50
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.93	0.50
1:A:392:LYS:HB3	3:A:1916:HOH:O	2.11	0.50
1:D:321:ASN:OD1	3:D:1754:HOH:O	2.19	0.50
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.92	0.50
1:B:41:LYS:HG3	3:B:986:HOH:O	2.12	0.50
1:D:40:ARG:HH11	1:D:40:ARG:CG	2.25	0.50
1:A:139:LYS:HD2	3:A:1532:HOH:O	2.12	0.50
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.76	0.50
1:C:658:ARG:HG2	1:C:661:TYR:CE2	2.45	0.50
1:D:435:GLN:OE1	1:D:437:SER:HB2	2.11	0.50
1:A:645:GLY:HA2	3:A:1050:HOH:O	2.11	0.50
1:C:489:LYS:HB3	1:C:489:LYS:HZ3	1.76	0.50
1:C:673:LEU:HD12	1:C:673:LEU:N	2.27	0.50
1:B:435:GLN:NE2	1:B:441:LYS:CD	2.74	0.50
1:B:459:VAL:HG22	1:B:460:SER:N	2.26	0.50
1:C:472:CYS:O	1:C:478:PRO:HA	2.11	0.50
1:C:57:LEU:HD23	3:C:1025:HOH:O	2.11	0.50
1:C:71:LYS:N	3:C:1251:HOH:O	2.44	0.50
1:B:741:GLY:O	1:B:742:ILE:C	2.50	0.50
1:C:158:SER:HB3	1:C:163:LYS:HB2	1.93	0.50
1:C:612:GLN:O	1:C:616:MET:HG3	2.12	0.50
1:D:673:LEU:HD12	1:D:673:LEU:N	2.27	0.50
1:A:361:GLU:CD	3:A:1015:HOH:O	2.50	0.50
1:B:622:LYS:NZ	3:B:1303:HOH:O	2.44	0.50
1:C:136:ASP:OD1	1:C:138:ASN:HB2	2.12	0.50
1:C:438:ASP:OD1	1:C:440:THR:HB	2.12	0.50
1:D:612:GLN:O	1:D:616:MET:HG3	2.12	0.50
1:D:74:ASN:C	1:D:92:ASN:HB3	2.32	0.50
1:D:521:GLU:HA	3:D:1395:HOH:O	2.10	0.49
1:A:285:ILE:N	1:A:285:ILE:HD13	2.27	0.49
1:A:516:PHE:CE2	1:A:523:LYS:HE2	2.47	0.49
1:B:658:ARG:O	1:B:658:ARG:HG3	2.12	0.49
1:D:306:ALA:CB	1:D:310:ARG:HD2	2.42	0.49
1:D:438:ASP:OD1	1:D:440:THR:HB	2.12	0.49
1:B:285:ILE:CD1	1:B:285:ILE:N	2.75	0.49
1:B:291:ALA:O	1:B:295:ILE:HG23	2.13	0.49
1:C:186:THR:HB	3:C:1474:HOH:O	2.12	0.49
1:C:278:SER:N	3:C:1462:HOH:O	2.45	0.49
1:D:136:ASP:OD1	1:D:138:ASN:HB2	2.11	0.49
1:B:622:LYS:NZ	1:B:622:LYS:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:VAL:HG23	1:C:161:GLY:H	1.78	0.49
1:D:504:LEU:HA	1:D:507:VAL:HG12	1.94	0.49
1:A:379:GLU:HB2	3:A:1810:HOH:O	2.11	0.49
1:A:513:LYS:HE3	1:A:530:LEU:HD11	1.94	0.49
1:B:651:ILE:HG21	1:B:755:MET:HE2	1.94	0.49
1:C:306:ALA:CB	1:C:310:ARG:HD2	2.43	0.49
1:B:341:VAL:O	1:B:342:ALA:CB	2.56	0.49
1:B:392:LYS:HD2	1:B:393:ASP:N	2.28	0.49
1:C:314:GLN:HG3	3:C:946:HOH:O	2.13	0.49
1:B:71:LYS:NZ	1:B:105:TYR:HB2	2.28	0.49
1:B:379:GLU:HG2	1:B:381:TYR:CD1	2.47	0.49
1:C:504:LEU:HA	1:C:507:VAL:HG12	1.95	0.49
1:D:173:TYR:HB3	1:D:182:SER:OG	2.13	0.49
1:D:481:THR:OG1	1:D:483:HIS:HE1	1.96	0.49
1:A:277:SER:O	1:A:278:SER:CB	2.61	0.49
1:C:74:ASN:C	1:C:92:ASN:HB3	2.33	0.49
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.94	0.49
1:D:276:LEU:HD23	1:D:276:LEU:O	2.12	0.49
1:D:718:GLN:HE21	1:D:718:GLN:HA	1.78	0.49
1:A:110:ASP:OD2	1:A:162:HIS:ND1	2.45	0.49
1:A:741:GLY:O	1:A:742:ILE:C	2.51	0.49
1:C:413:ASP:HB3	1:C:414:TYR:CD1	2.48	0.49
1:C:435:GLN:OE1	1:C:437:SER:HB2	2.11	0.49
1:C:139:LYS:HD3	3:C:1349:HOH:O	2.12	0.48
1:D:140:ARG:NH1	1:D:140:ARG:HG2	2.27	0.48
1:D:39:SER:O	1:D:40:ARG:O	2.31	0.48
1:D:697:GLN:HG3	3:D:1792:HOH:O	2.11	0.48
1:A:147:ARG:HG2	3:A:1675:HOH:O	2.12	0.48
1:B:276:LEU:N	1:B:276:LEU:CD2	2.74	0.48
1:C:523:LYS:HG2	3:C:876:HOH:O	2.12	0.48
1:D:377:ASN:HB2	1:D:381:TYR:O	2.12	0.48
1:D:528:MET:HE3	1:D:530:LEU:CD2	2.34	0.48
1:D:741:GLY:O	1:D:742:ILE:C	2.51	0.48
1:A:39:SER:O	1:A:40:ARG:O	2.31	0.48
1:B:98:PHE:CE2	1:B:100:HIS:HB2	2.48	0.48
1:C:102:ILE:HD13	1:C:116:LEU:HD22	1.94	0.48
1:D:60:LEU:C	1:D:60:LEU:HD12	2.34	0.48
1:A:704:HIS:HE1	1:A:711:VAL:O	1.96	0.48
1:C:172:ILE:H	1:C:186:THR:CG2	2.23	0.48
1:C:276:LEU:O	1:C:276:LEU:HD23	2.12	0.48
1:D:93:SER:HA	1:D:96:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ALA:HA	3:A:849:HOH:O	2.11	0.48
1:B:481:THR:OG1	1:B:483:HIS:HE1	1.96	0.48
1:C:458:SER:OG	1:C:471:ARG:HB2	2.13	0.48
1:C:74:ASN:HB3	1:C:92:ASN:HB3	1.96	0.48
1:D:136:ASP:CG	1:D:139:LYS:HG2	2.34	0.48
1:A:140:ARG:HH11	1:A:140:ARG:CG	2.19	0.48
1:A:71:LYS:NZ	1:A:105:TYR:HB2	2.28	0.48
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.49	0.48
1:B:137:LEU:O	1:B:140:ARG:NH1	2.46	0.48
1:C:40:ARG:HH11	1:C:40:ARG:CG	2.26	0.48
1:C:481:THR:OG1	1:C:483:HIS:HE1	1.97	0.48
1:D:413:ASP:HB3	1:D:414:TYR:CD1	2.48	0.48
1:D:415:LEU:HD13	1:D:415:LEU:C	2.34	0.48
1:D:98:PHE:CE2	1:D:100:HIS:HB2	2.49	0.48
1:A:291:ALA:O	1:A:295:ILE:HG23	2.13	0.48
1:D:160:VAL:HG23	1:D:161:GLY:H	1.77	0.48
1:B:39:SER:O	1:B:40:ARG:O	2.31	0.48
1:B:704:HIS:HE1	1:B:711:VAL:O	1.95	0.48
1:C:140:ARG:NH1	1:C:140:ARG:HG2	2.27	0.48
1:B:187:TRP:N	1:B:187:TRP:CD1	2.81	0.48
1:B:276:LEU:HD22	1:B:276:LEU:H	1.79	0.48
1:B:379:GLU:HG3	3:B:1626:HOH:O	2.12	0.48
1:B:435:GLN:NE2	1:B:441:LYS:HD2	2.29	0.48
1:B:61:ARG:NH1	3:B:1551:HOH:O	2.45	0.48
1:C:98:PHE:CE2	1:C:100:HIS:HB2	2.49	0.48
1:D:505:GLN:HB3	3:D:1471:HOH:O	2.13	0.48
1:D:74:ASN:HB3	1:D:92:ASN:CB	2.43	0.48
1:A:137:LEU:O	1:A:140:ARG:NH1	2.46	0.47
1:C:173:TYR:HB3	1:C:182:SER:OG	2.14	0.47
1:C:520:ASN:HA	3:C:1515:HOH:O	2.13	0.47
1:C:615:LYS:NZ	3:C:1144:HOH:O	2.38	0.47
1:D:459:VAL:HG22	1:D:460:SER:N	2.29	0.47
1:D:74:ASN:HB3	1:D:92:ASN:HB3	1.95	0.47
1:A:71:LYS:HE3	3:A:1782:HOH:O	2.14	0.47
1:B:253:ARG:HG3	3:B:1727:HOH:O	2.14	0.47
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.44	0.47
1:D:272:ASN:HD22	1:D:273:THR:N	2.12	0.47
1:A:97:GLU:HG2	3:A:1217:HOH:O	2.14	0.47
1:C:60:LEU:HD12	1:C:60:LEU:C	2.34	0.47
1:C:74:ASN:HB3	1:C:92:ASN:CB	2.43	0.47
1:D:51:ASN:HA	3:D:1204:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TRP:N	1:A:187:TRP:CD1	2.81	0.47
1:A:658:ARG:HG2	1:A:661:TYR:CD2	2.49	0.47
1:B:358:ARG:NH2	3:B:1305:HOH:O	2.46	0.47
1:C:272:ASN:HD21	1:C:274:ASP:HB2	1.79	0.47
1:C:272:ASN:HD22	1:C:273:THR:N	2.11	0.47
1:C:343:ARG:HD2	3:C:1044:HOH:O	2.13	0.47
1:C:691:ARG:NE	3:C:1662:HOH:O	2.30	0.47
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.79	0.47
1:A:281:ASN:HB3	3:A:1866:HOH:O	2.15	0.47
1:B:764:SER:HA	3:B:1050:HOH:O	2.14	0.47
1:C:741:GLY:O	1:C:742:ILE:C	2.52	0.47
1:C:76:ILE:CD1	1:C:90:LEU:HD11	2.39	0.47
1:D:102:ILE:HD13	1:D:116:LEU:HD22	1.95	0.47
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.50	0.47
1:D:726:VAL:O	1:D:726:VAL:HG13	2.15	0.47
1:A:580:GLY:O	1:A:583:SER:HB2	2.15	0.47
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.35	0.47
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.44	0.47
1:A:85:ASN:ND2	3:A:1859:HOH:O	2.47	0.47
1:B:277:SER:O	1:B:278:SER:CB	2.61	0.47
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.50	0.47
1:B:71:LYS:HZ1	1:B:105:TYR:HB2	1.79	0.47
1:C:276:LEU:N	1:C:276:LEU:CD2	2.75	0.47
1:C:40:ARG:HB2	1:C:506:ASN:O	2.15	0.47
1:A:392:LYS:HD2	1:A:393:ASP:N	2.29	0.47
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.96	0.47
1:D:422:TYR:CD2	1:D:423:LYS:HD3	2.50	0.47
1:D:40:ARG:HB2	1:D:506:ASN:O	2.14	0.47
1:C:40:ARG:NH1	1:C:505:GLN:O	2.47	0.47
1:C:429:ARG:NE	3:C:865:HOH:O	2.39	0.47
1:A:358:ARG:NH1	3:A:1346:HOH:O	2.46	0.47
1:D:272:ASN:HD21	1:D:274:ASP:HB2	1.80	0.47
1:A:407:ILE:CG2	1:A:415:LEU:HD21	2.45	0.47
1:A:276:LEU:H	1:A:276:LEU:HD22	1.78	0.47
1:A:74:ASN:HB3	1:A:92:ASN:CG	2.35	0.47
1:C:136:ASP:CG	1:C:139:LYS:HG2	2.35	0.47
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.79	0.47
1:C:93:SER:HA	1:C:96:ASP:OD1	2.14	0.47
1:D:483:HIS:HD2	3:D:1104:HOH:O	1.98	0.47
1:D:502:LYS:HD3	3:D:1101:HOH:O	2.15	0.47
1:A:140:ARG:CG	1:A:140:ARG:NH1	2.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LYS:HB2	3:A:788:HOH:O	2.15	0.46
1:B:472:CYS:O	1:B:478:PRO:HA	2.15	0.46
1:D:458:SER:OG	1:D:471:ARG:HB2	2.15	0.46
1:A:366:LEU:HB3	3:A:1020:HOH:O	2.15	0.46
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.31	0.46
1:B:140:ARG:HH11	1:B:140:ARG:CG	2.19	0.46
1:B:310:ARG:NH1	1:B:329:ASP:OD1	2.49	0.46
1:B:726:VAL:O	1:B:726:VAL:CG1	2.63	0.46
1:C:459:VAL:HG22	1:C:460:SER:N	2.30	0.46
1:C:489:LYS:HG3	3:C:821:HOH:O	2.15	0.46
1:D:341:VAL:C	1:D:343:ARG:H	2.19	0.46
1:D:691:ARG:NE	3:D:1753:HOH:O	2.26	0.46
1:A:310:ARG:CZ	3:A:1515:HOH:O	2.61	0.46
1:C:354:VAL:HG12	3:C:1500:HOH:O	2.14	0.46
1:A:341:VAL:C	1:A:343:ARG:H	2.19	0.46
1:A:342:ALA:CB	3:A:1804:HOH:O	2.62	0.46
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.51	0.46
1:B:523:LYS:HD3	3:B:1814:HOH:O	2.15	0.46
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.51	0.46
1:C:271:VAL:HG23	1:C:283:THR:O	2.16	0.46
1:C:528:MET:HE3	1:C:530:LEU:CD2	2.35	0.46
1:D:69:LEU:HD11	1:D:107:ILE:HD12	1.96	0.46
1:B:159:PRO:HG3	3:B:1103:HOH:O	2.16	0.46
1:C:147:ARG:HD3	3:C:1473:HOH:O	2.15	0.46
1:C:415:LEU:HD13	1:C:415:LEU:C	2.36	0.46
1:C:538:LYS:HA	3:C:1265:HOH:O	2.15	0.46
1:B:74:ASN:HB3	1:B:92:ASN:CG	2.36	0.46
1:C:402:TRP:CD2	1:C:421:GLU:HB2	2.50	0.46
1:D:358:ARG:NH2	3:D:951:HOH:O	2.48	0.46
1:D:382:ARG:NH2	3:D:802:HOH:O	2.47	0.46
1:A:435:GLN:HE22	1:A:441:LYS:CD	2.27	0.46
1:A:74:ASN:HB2	3:A:1680:HOH:O	2.14	0.46
1:B:41:LYS:HB2	3:B:1110:HOH:O	2.16	0.46
1:C:341:VAL:C	1:C:343:ARG:H	2.19	0.46
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.45	0.46
1:A:616:MET:HE1	3:A:1894:HOH:O	2.16	0.46
1:B:407:ILE:CG2	1:B:415:LEU:HD21	2.46	0.46
1:D:271:VAL:HG23	1:D:283:THR:O	2.15	0.46
1:D:397:ILE:HG13	1:D:398:THR:HG23	1.98	0.46
1:A:276:LEU:H	1:A:276:LEU:HD23	1.80	0.46
1:C:69:LEU:HD11	1:C:107:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LYS:HE2	3:C:1224:HOH:O	2.15	0.46
1:C:388:GLN:CB	1:C:391:LYS:HB2	2.46	0.46
1:C:85:ASN:ND2	3:C:1021:HOH:O	2.49	0.46
1:D:160:VAL:HG21	3:D:1571:HOH:O	2.15	0.46
1:D:173:TYR:CE2	1:D:184:ARG:HG3	2.51	0.46
1:D:764:SER:HB2	3:D:1325:HOH:O	2.16	0.46
1:A:186:THR:HG21	1:A:196:ASN:CB	2.46	0.45
1:A:454:CYS:HB2	3:A:1607:HOH:O	2.16	0.45
1:A:98:PHE:CD2	1:A:100:HIS:HB2	2.52	0.45
1:B:140:ARG:NH1	1:B:140:ARG:CG	2.76	0.45
1:B:562:ASN:HB2	3:B:826:HOH:O	2.17	0.45
1:D:334:SER:HB3	1:D:336:ARG:CD	2.46	0.45
1:A:546:VAL:HG22	1:A:547:TYR:N	2.31	0.45
1:A:721:LYS:HD3	1:B:736:THR:HG23	1.98	0.45
1:B:662:TYR:CE2	2:B:800:AAF:H132	2.51	0.45
1:C:310:ARG:HG3	1:C:329:ASP:OD1	2.16	0.45
1:C:79:PHE:CD1	1:C:86:SER:HB3	2.51	0.45
1:D:276:LEU:N	1:D:276:LEU:CD2	2.74	0.45
1:D:40:ARG:NH1	1:D:505:GLN:O	2.50	0.45
1:B:341:VAL:C	1:B:343:ARG:H	2.19	0.45
1:C:154:TRP:CE2	1:C:212:SER:HB2	2.50	0.45
1:C:186:THR:HG21	1:C:196:ASN:CB	2.47	0.45
1:D:186:THR:HG21	1:D:196:ASN:CB	2.47	0.45
1:D:498:SER:O	1:D:502:LYS:HG2	2.17	0.45
1:A:161:GLY:HA3	3:A:1154:HOH:O	2.17	0.45
1:A:71:LYS:HE2	1:A:76:ILE:CD1	2.47	0.45
1:B:546:VAL:HG22	1:B:547:TYR:N	2.30	0.45
1:B:71:LYS:HE2	1:B:76:ILE:CD1	2.46	0.45
1:D:310:ARG:HG3	1:D:329:ASP:OD1	2.16	0.45
1:D:413:ASP:HB3	1:D:414:TYR:HD1	1.82	0.45
1:A:114:ILE:HD11	1:A:137:LEU:HD11	1.98	0.45
1:A:61:ARG:HG3	3:A:1672:HOH:O	2.17	0.45
1:B:325:MET:HE2	1:B:327:ILE:HG12	1.97	0.45
1:B:761:GLN:HB3	1:B:761:GLN:HE21	1.66	0.45
1:B:80:ASN:HB2	3:B:1465:HOH:O	2.17	0.45
1:D:147:ARG:HD3	3:D:1078:HOH:O	2.15	0.45
1:D:489:LYS:HZ3	1:D:489:LYS:HB3	1.79	0.45
1:D:79:PHE:CD1	1:D:86:SER:HB3	2.51	0.45
1:A:415:LEU:C	1:A:415:LEU:HD13	2.36	0.45
1:C:455:GLN:HA	3:C:1575:HOH:O	2.16	0.45
1:C:173:TYR:CE2	1:C:184:ARG:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:SER:HB3	1:C:336:ARG:CD	2.46	0.45
1:C:658:ARG:HD2	1:C:661:TYR:CE1	2.51	0.45
1:C:649:CYS:HB3	1:C:699:GLU:HB2	1.99	0.45
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.52	0.45
1:C:253:ARG:HH22	1:D:253:ARG:HH22	1.64	0.45
1:C:512:LYS:HD3	3:C:948:HOH:O	2.16	0.45
1:B:110:ASP:HB3	1:B:112:GLN:HB2	1.99	0.45
1:D:388:GLN:CB	1:D:391:LYS:HB2	2.47	0.45
1:A:310:ARG:NH1	1:A:329:ASP:OD1	2.50	0.45
1:B:310:ARG:CZ	3:B:1167:HOH:O	2.65	0.45
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.47	0.45
1:B:579:ASP:HB3	1:B:583:SER:OG	2.17	0.45
1:D:306:ALA:HB3	1:D:310:ARG:HD2	1.98	0.45
1:B:186:THR:HG21	1:B:196:ASN:CB	2.47	0.44
1:B:50:LYS:HE3	3:B:1636:HOH:O	2.16	0.44
1:D:147:ARG:NH1	3:D:1473:HOH:O	2.50	0.44
1:B:107:ILE:HG12	1:B:114:ILE:HG12	1.99	0.44
1:B:276:LEU:HD23	1:B:276:LEU:H	1.80	0.44
1:B:697:GLN:NE2	3:B:1646:HOH:O	2.39	0.44
1:C:141:GLN:HA	3:C:1319:HOH:O	2.16	0.44
1:C:513:LYS:O	1:C:527:GLN:HA	2.17	0.44
1:A:442:VAL:HG11	3:A:1768:HOH:O	2.17	0.44
1:A:504:LEU:HA	1:A:507:VAL:CG1	2.48	0.44
1:D:513:LYS:O	1:D:527:GLN:HA	2.17	0.44
1:D:704:HIS:HE1	1:D:711:VAL:O	2.00	0.44
1:A:231:THR:HG22	1:A:232:GLU:HG3	2.00	0.44
1:A:651:ILE:HG21	1:A:755:MET:HE2	1.99	0.44
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.46	0.44
1:A:726:VAL:O	1:A:726:VAL:CG1	2.64	0.44
1:B:136:ASP:OD1	1:B:138:ASN:HB2	2.17	0.44
1:B:580:GLY:O	1:B:583:SER:HB2	2.17	0.44
1:D:492:ARG:HA	3:D:1752:HOH:O	2.17	0.44
1:A:489:LYS:HZ2	1:A:489:LYS:HB3	1.81	0.44
1:B:114:ILE:HD11	1:B:137:LEU:HD11	1.99	0.44
1:B:377:ASN:ND2	3:B:827:HOH:O	2.49	0.44
1:B:717:ALA:HA	3:B:1870:HOH:O	2.17	0.44
1:C:498:SER:O	1:C:502:LYS:HG2	2.17	0.44
1:B:415:LEU:HD13	1:B:415:LEU:C	2.38	0.44
1:C:108:SER:C	1:C:110:ASP:N	2.71	0.44
1:C:397:ILE:HG13	1:C:398:THR:HG23	1.99	0.44
1:C:704:HIS:HE1	1:C:711:VAL:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:726:VAL:O	1:C:726:VAL:HG13	2.17	0.44
1:D:471:ARG:HG2	1:D:480:TYR:CD2	2.53	0.44
1:A:152:THR:HG21	1:A:155:VAL:CG2	2.48	0.44
1:A:471:ARG:HG3	3:A:1510:HOH:O	2.18	0.44
1:B:152:THR:HG21	1:B:155:VAL:CG2	2.47	0.44
1:C:471:ARG:HG2	1:C:480:TYR:CD2	2.53	0.44
1:C:734:TRP:CD1	1:C:736:THR:HG22	2.53	0.44
1:D:319:ILE:HD11	1:D:673:LEU:CD1	2.48	0.44
1:D:388:GLN:HG2	1:D:391:LYS:HD3	2.00	0.44
1:D:658:ARG:HD2	1:D:661:TYR:CE1	2.52	0.44
1:B:106:SER:HB3	1:B:115:LEU:HB3	2.00	0.43
1:C:306:ALA:HB3	1:C:310:ARG:HD2	1.99	0.43
1:C:321:ASN:ND2	3:C:1389:HOH:O	2.50	0.43
1:C:697:GLN:HG3	3:C:1475:HOH:O	2.18	0.43
1:D:172:ILE:H	1:D:186:THR:CG2	2.24	0.43
1:D:243:ASP:HB3	3:D:1071:HOH:O	2.17	0.43
1:D:343:ARG:NH2	3:D:905:HOH:O	2.49	0.43
1:D:505:GLN:HB3	3:D:822:HOH:O	2.19	0.43
1:D:78:VAL:HG13	1:D:78:VAL:O	2.18	0.43
1:A:107:ILE:HG12	1:A:114:ILE:HG12	2.00	0.43
1:A:377:ASN:HB3	1:A:379:GLU:H	1.82	0.43
1:B:336:ARG:HG3	1:B:336:ARG:H	1.65	0.43
1:B:489:LYS:HB3	1:B:489:LYS:HZ2	1.83	0.43
1:C:184:ARG:HD2	1:C:187:TRP:CD2	2.52	0.43
1:C:516:PHE:CE2	1:C:523:LYS:HE2	2.53	0.43
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.46	0.43
1:D:52:THR:HG22	3:D:1187:HOH:O	2.18	0.43
1:D:697:GLN:HG3	3:D:1488:HOH:O	2.17	0.43
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.53	0.43
1:C:388:GLN:HG2	1:C:391:LYS:HD3	2.00	0.43
1:D:546:VAL:HG22	1:D:547:TYR:N	2.33	0.43
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.53	0.43
1:B:435:GLN:NE2	1:B:441:LYS:HD3	2.34	0.43
1:B:609:ALA:HA	3:B:1143:HOH:O	2.17	0.43
1:D:310:ARG:NH1	1:D:329:ASP:OD1	2.52	0.43
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.43
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.99	0.43
1:B:487:ASN:O	1:B:488:ASP:HB2	2.17	0.43
1:C:413:ASP:HB3	1:C:414:TYR:HD1	1.82	0.43
1:C:721:LYS:NZ	3:C:1313:HOH:O	2.51	0.43
1:C:89:PHE:CD1	1:C:90:LEU:HD12	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ARG:HD2	3:D:1523:HOH:O	2.18	0.43
1:D:98:PHE:CD2	1:D:100:HIS:HB2	2.53	0.43
1:A:110:ASP:HB3	1:A:112:GLN:HB2	1.99	0.43
1:C:319:ILE:HD11	1:C:673:LEU:CD1	2.48	0.43
1:C:98:PHE:CD2	1:C:100:HIS:HB2	2.53	0.43
1:D:520:ASN:O	1:D:521:GLU:HB2	2.19	0.43
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.54	0.43
1:B:183:TYR:HE1	1:B:277:SER:C	2.22	0.43
1:B:377:ASN:HB3	1:B:379:GLU:H	1.83	0.43
1:C:147:ARG:HB2	3:C:1018:HOH:O	2.19	0.43
1:C:310:ARG:NH1	1:C:329:ASP:OD1	2.52	0.43
1:C:546:VAL:HG22	1:C:547:TYR:N	2.34	0.43
1:C:718:GLN:HE21	1:C:718:GLN:HA	1.84	0.43
1:A:253:ARG:HG3	3:A:1821:HOH:O	2.18	0.43
1:B:177:GLU:CB	1:B:180:LEU:HD22	2.41	0.43
1:B:435:GLN:HE22	1:B:441:LYS:CD	2.32	0.43
1:D:92:ASN:HA	3:D:1633:HOH:O	2.19	0.43
1:A:187:TRP:CZ2	3:A:1866:HOH:O	2.72	0.42
1:A:472:CYS:O	1:A:478:PRO:HA	2.19	0.42
1:B:388:GLN:HB2	3:B:1831:HOH:O	2.18	0.42
1:B:536:LYS:HB3	1:B:536:LYS:NZ	2.34	0.42
1:C:183:TYR:CE2	1:C:276:LEU:HG	2.54	0.42
1:C:237:GLU:HA	1:C:252:VAL:O	2.20	0.42
1:C:289:ALA:CB	1:C:290:PRO:HA	2.25	0.42
1:C:379:GLU:HG2	3:C:1061:HOH:O	2.19	0.42
1:C:422:TYR:CZ	1:C:423:LYS:HE3	2.54	0.42
1:C:503:MET:HE3	3:C:1625:HOH:O	2.18	0.42
1:D:492:ARG:HD3	3:D:889:HOH:O	2.19	0.42
1:A:106:SER:HB3	1:A:115:LEU:HB3	2.00	0.42
1:A:487:ASN:O	1:A:488:ASP:HB2	2.19	0.42
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.53	0.42
1:C:111:GLY:O	1:C:137:LEU:HD12	2.19	0.42
1:C:319:ILE:C	1:C:321:ASN:H	2.22	0.42
1:C:520:ASN:O	1:C:521:GLU:HB2	2.19	0.42
1:C:78:VAL:O	1:C:78:VAL:HG13	2.20	0.42
1:D:415:LEU:HB3	1:D:434:ILE:CG2	2.49	0.42
1:A:458:SER:OG	1:A:471:ARG:HB2	2.19	0.42
1:A:403:GLU:OE1	1:A:585:TYR:HA	2.20	0.42
1:B:630:SER:HA	1:B:654:ALA:O	2.20	0.42
1:D:184:ARG:HD2	1:D:187:TRP:CD2	2.53	0.42
1:D:517:ILE:HA	3:D:1680:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:GLU:OE1	1:D:585:TYR:HA	2.20	0.42
1:A:536:LYS:HB3	1:A:536:LYS:NZ	2.33	0.42
1:B:331:ASP:HB3	1:B:334:SER:HB2	2.01	0.42
1:C:334:SER:CB	1:C:336:ARG:HD2	2.49	0.42
1:C:513:LYS:HE3	3:C:1577:HOH:O	2.18	0.42
1:C:660:GLU:HG3	3:C:800:HOH:O	2.20	0.42
1:D:336:ARG:H	1:D:336:ARG:HD2	1.85	0.42
1:A:136:ASP:OD1	1:A:138:ASN:HB2	2.19	0.42
1:B:175:LYS:NZ	3:B:1555:HOH:O	2.51	0.42
1:B:528:MET:HB2	1:B:528:MET:HE2	1.93	0.42
1:B:533:HIS:HD2	3:B:1851:HOH:O	2.00	0.42
1:B:691:ARG:NH2	3:B:1749:HOH:O	2.53	0.42
1:C:54:ARG:HB2	1:C:54:ARG:HE	1.69	0.42
1:D:111:GLY:O	1:D:137:LEU:HD12	2.19	0.42
1:D:40:ARG:HE	1:D:508:GLN:HG2	1.85	0.42
1:D:734:TRP:CD1	1:D:736:THR:HG22	2.54	0.42
1:A:334:SER:HB3	1:A:336:ARG:CD	2.50	0.42
1:B:334:SER:HB3	1:B:336:ARG:CD	2.50	0.42
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.95	0.42
1:B:532:PRO:HD3	1:B:569:SER:HA	2.02	0.42
1:C:268:PHE:CD2	1:C:313:LEU:HD21	2.54	0.42
1:C:536:LYS:NZ	1:C:536:LYS:CB	2.83	0.42
1:D:358:ARG:NE	3:D:1587:HOH:O	2.52	0.42
1:B:247:GLN:NE2	3:B:1915:HOH:O	2.52	0.42
1:B:658:ARG:HB3	1:B:689:MET:HE1	2.02	0.42
1:C:336:ARG:HD2	1:C:336:ARG:H	1.85	0.42
1:D:334:SER:CB	1:D:336:ARG:HD2	2.49	0.42
1:D:375:ILE:HB	3:D:1766:HOH:O	2.18	0.42
1:D:486:VAL:CG1	1:D:487:ASN:N	2.82	0.42
1:D:718:GLN:NE2	1:D:718:GLN:HA	2.35	0.42
1:A:579:ASP:HB3	1:A:583:SER:OG	2.20	0.42
1:B:231:THR:HG22	1:B:232:GLU:HG3	2.02	0.42
1:C:342:ALA:HA	3:C:1288:HOH:O	2.20	0.42
1:C:415:LEU:HB3	1:C:434:ILE:CG2	2.50	0.42
1:D:183:TYR:CE2	1:D:276:LEU:HG	2.54	0.42
1:D:505:GLN:HB2	3:D:1750:HOH:O	2.19	0.42
1:D:57:LEU:HB3	3:D:1319:HOH:O	2.19	0.42
1:A:183:TYR:HE1	1:A:277:SER:C	2.23	0.41
1:A:282:ALA:HB1	3:A:1288:HOH:O	2.19	0.41
1:A:561:LEU:HA	1:A:561:LEU:HD12	1.92	0.41
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ALA:HB3	3:C:1103:HOH:O	2.18	0.41
1:C:679:ASN:ND2	3:C:1017:HOH:O	2.53	0.41
1:D:108:SER:C	1:D:110:ASP:N	2.71	0.41
1:D:65:ASP:CG	1:D:464:GLU:HB2	2.40	0.41
1:A:177:GLU:CB	1:A:180:LEU:HD22	2.43	0.41
1:A:512:LYS:HD3	3:A:1077:HOH:O	2.20	0.41
1:B:704:HIS:CE1	1:B:711:VAL:O	2.73	0.41
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.55	0.41
1:C:40:ARG:HE	1:C:508:GLN:HG2	1.85	0.41
1:C:65:ASP:CG	1:C:464:GLU:HB2	2.40	0.41
1:D:422:TYR:CZ	1:D:423:LYS:HE3	2.55	0.41
1:D:54:ARG:HE	1:D:54:ARG:HB2	1.69	0.41
1:D:89:PHE:CD1	1:D:90:LEU:HD12	2.35	0.41
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.56	0.41
1:A:532:PRO:HD3	1:A:569:SER:HA	2.02	0.41
1:B:366:LEU:HD12	3:B:1691:HOH:O	2.21	0.41
1:B:543:LEU:HD12	1:B:567:LEU:HD13	2.02	0.41
1:C:615:LYS:HG2	3:C:1144:HOH:O	2.21	0.41
1:B:218:PRO:HB2	1:B:308:GLN:NE2	2.36	0.41
1:C:388:GLN:HB2	1:C:391:LYS:HB2	2.02	0.41
1:D:283:THR:HG22	1:D:285:ILE:HD12	2.03	0.41
1:D:289:ALA:CB	1:D:290:PRO:CA	2.89	0.41
1:C:91:GLU:HB2	3:C:1085:HOH:O	2.21	0.41
1:A:175:LYS:HE3	1:A:180:LEU:O	2.21	0.41
1:B:160:VAL:CG2	1:B:161:GLY:N	2.83	0.41
1:B:60:LEU:C	1:B:60:LEU:HD12	2.41	0.41
1:C:542:LEU:HD23	1:C:542:LEU:C	2.41	0.41
1:C:392:LYS:HB3	3:C:1446:HOH:O	2.19	0.41
1:C:658:ARG:HD2	1:C:661:TYR:CZ	2.56	0.41
1:D:319:ILE:C	1:D:321:ASN:H	2.21	0.41
1:D:388:GLN:HB2	1:D:391:LYS:HB2	2.03	0.41
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.55	0.41
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.56	0.41
1:C:358:ARG:NH2	3:C:943:HOH:O	2.52	0.41
1:C:487:ASN:HB2	3:C:821:HOH:O	2.20	0.41
1:D:268:PHE:CD2	1:D:313:LEU:HD21	2.55	0.41
1:D:384:ILE:HG13	1:D:404:VAL:HG21	2.02	0.41
1:D:536:LYS:CB	1:D:536:LYS:NZ	2.84	0.41
1:A:40:ARG:NH1	3:A:1508:HOH:O	2.54	0.41
1:A:82:GLU:HG2	1:A:83:TYR:CZ	2.55	0.41
1:B:76:ILE:HB	1:B:90:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:GLU:OE2	1:C:253:ARG:NH2	2.47	0.41
1:D:285:ILE:HD12	1:D:285:ILE:N	2.36	0.41
1:A:276:LEU:HD23	1:A:276:LEU:O	2.21	0.41
1:A:537:SER:O	1:C:350:THR:HB	2.20	0.41
1:A:691:ARG:NE	3:A:1911:HOH:O	2.21	0.41
1:B:71:LYS:HE2	1:B:76:ILE:HD13	2.03	0.41
1:B:82:GLU:HG2	1:B:83:TYR:CZ	2.56	0.41
1:C:147:ARG:HG2	1:C:147:ARG:HH11	1.86	0.41
1:C:630:SER:OG	3:C:1661:HOH:O	2.20	0.41
1:D:429:ARG:NE	3:D:876:HOH:O	2.48	0.41
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.02	0.41
1:A:331:ASP:HB3	1:A:334:SER:HB2	2.02	0.41
1:A:60:LEU:HD12	1:A:60:LEU:C	2.41	0.41
1:A:685:ASN:ND2	3:A:1196:HOH:O	2.51	0.41
1:B:175:LYS:HE3	1:B:180:LEU:O	2.21	0.41
1:B:325:MET:HE1	1:B:327:ILE:HD11	2.02	0.41
1:B:78:VAL:O	1:B:78:VAL:HG13	2.20	0.41
1:C:384:ILE:HG13	1:C:404:VAL:HG21	2.02	0.41
1:A:409:ALA:O	1:A:415:LEU:HD22	2.21	0.40
1:A:704:HIS:CE1	1:A:711:VAL:O	2.73	0.40
1:B:369:ASN:ND2	3:B:1167:HOH:O	2.53	0.40
1:C:283:THR:HG22	1:C:285:ILE:HD12	2.02	0.40
1:D:489:LYS:HG3	3:D:1169:HOH:O	2.20	0.40
1:D:726:VAL:O	1:D:726:VAL:CG1	2.69	0.40
1:A:413:ASP:HB3	1:A:414:TYR:CD1	2.56	0.40
1:B:155:VAL:HG22	1:B:166:TYR:HB2	2.03	0.40
1:D:160:VAL:O	1:D:161:GLY:O	2.39	0.40
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.96	0.40
1:A:90:LEU:HD22	1:A:91:GLU:O	2.22	0.40
1:B:158:SER:HB3	1:B:163:LYS:HB2	2.04	0.40
1:B:411:THR:HG21	3:B:1314:HOH:O	2.20	0.40
1:D:507:VAL:HB	3:D:1760:HOH:O	2.21	0.40
1:D:85:ASN:ND2	3:D:1371:HOH:O	2.50	0.40
1:A:217:SER:HB3	1:A:222:PHE:HB2	2.03	0.40
1:A:543:LEU:HD12	1:A:567:LEU:HD13	2.03	0.40
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.56	0.40
1:D:658:ARG:HD2	1:D:661:TYR:CZ	2.56	0.40
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.70	0.40
1:A:156:THR:CG2	1:A:214:LEU:HD11	2.52	0.40
1:A:513:LYS:O	1:A:527:GLN:HA	2.22	0.40
1:A:693:GLU:HB2	3:A:965:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:SER:C	1:C:110:ASP:H	2.25	0.40
1:C:630:SER:HA	1:C:654:ALA:O	2.21	0.40
1:C:696:LYS:NZ	3:C:1402:HOH:O	2.54	0.40
1:C:81:ALA:O	1:C:492:ARG:NH2	2.54	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	724/726 (100%)	678 (94%)	39 (5%)	7 (1%)	18	10
1	B	724/726 (100%)	678 (94%)	39 (5%)	7 (1%)	18	10
1	C	724/726 (100%)	677 (94%)	40 (6%)	7 (1%)	18	10
1	D	724/726 (100%)	676 (93%)	41 (6%)	7 (1%)	18	10
All	All	2896/2904 (100%)	2709 (94%)	159 (6%)	28 (1%)	18	10

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	278	SER
1	B	40	ARG
1	B	278	SER
1	C	40	ARG
1	C	278	SER
1	D	40	ARG
1	D	278	SER
1	A	161	GLY
1	A	289	ALA
1	B	161	GLY

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Mol	Chain	Res	Type
1	B	289	ALA
1	C	161	GLY
1	C	289	ALA
1	C	320	GLN
1	D	161	GLY
1	D	289	ALA
1	D	320	GLN
1	A	520	ASN
1	B	520	ASN
1	A	320	GLN
1	B	320	GLN
1	C	520	ASN
1	D	520	ASN
1	C	334	SER
1	D	334	SER
1	A	94	THR
1	B	94	THR

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	651/651 (100%)	603 (93%)	48 (7%)	16	10
1	B	651/651 (100%)	605 (93%)	46 (7%)	17	11
1	C	651/651 (100%)	609 (94%)	42 (6%)	20	14
1	D	651/651 (100%)	610 (94%)	41 (6%)	21	15
All	All	2604/2604 (100%)	2427 (93%)	177 (7%)	18	13

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	41	LYS
1	A	51	ASN

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Mol	Chain	Res	Type
1	A	57	LEU
1	A	66	HIS
1	A	73	GLU
1	A	90	LEU
1	A	91	GLU
1	A	92	ASN
1	A	110	ASP
1	A	140	ARG
1	A	141	GLN
1	A	170	ASN
1	A	207	VAL
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	272	ASN
1	A	276	LEU
1	A	285	ILE
1	A	303	VAL
1	A	313	LEU
1	A	336	ARG
1	A	358	ARG
1	A	361	GLU
1	A	385	CYS
1	A	388	GLN
1	A	392	LYS
1	A	413	ASP
1	A	436	LEU
1	A	440	THR
1	A	448	GLU
1	A	482	LEU
1	A	514	LEU
1	A	520	ASN
1	A	523	LYS
1	A	536	LYS
1	A	543	LEU
1	A	561	LEU
1	A	583	SER
1	A	603	VAL
1	A	658	ARG
1	A	673	LEU
1	A	679	ASN
1	A	701	LEU

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Mol	Chain	Res	Type
1	A	702	LEU
1	A	761	GLN
1	B	39	SER
1	B	40	ARG
1	B	41	LYS
1	B	51	ASN
1	B	57	LEU
1	B	66	HIS
1	B	73	GLU
1	B	90	LEU
1	B	91	GLU
1	B	92	ASN
1	B	110	ASP
1	B	140	ARG
1	B	141	GLN
1	B	170	ASN
1	B	207	VAL
1	B	246	LEU
1	B	253	ARG
1	B	254	VAL
1	B	272	ASN
1	B	276	LEU
1	B	285	ILE
1	B	313	LEU
1	B	336	ARG
1	B	361	GLU
1	B	385	CYS
1	B	388	GLN
1	B	392	LYS
1	B	413	ASP
1	B	436	LEU
1	B	440	THR
1	B	448	GLU
1	B	482	LEU
1	B	514	LEU
1	B	520	ASN
1	B	523	LYS
1	B	536	LYS
1	B	543	LEU
1	B	561	LEU
1	B	583	SER
1	B	603	VAL

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Mol	Chain	Res	Type
1	B	658	ARG
1	B	673	LEU
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	761	GLN
1	C	40	ARG
1	C	41	LYS
1	C	51	ASN
1	C	73	GLU
1	C	90	LEU
1	C	110	ASP
1	C	145	GLU
1	C	160	VAL
1	C	170	ASN
1	C	207	VAL
1	C	246	LEU
1	C	253	ARG
1	C	254	VAL
1	C	272	ASN
1	C	276	LEU
1	C	303	VAL
1	C	326	ASP
1	C	332	GLU
1	C	336	ARG
1	C	385	CYS
1	C	388	GLN
1	C	392	LYS
1	C	436	LEU
1	C	440	THR
1	C	448	GLU
1	C	482	LEU
1	C	505	GLN
1	C	514	LEU
1	C	523	LYS
1	C	536	LYS
1	C	543	LEU
1	C	561	LEU
1	C	566	TYR
1	C	583	SER
1	C	603	VAL
1	C	658	ARG

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Mol	Chain	Res	Type
1	C	679	ASN
1	C	689	MET
1	C	701	LEU
1	C	702	LEU
1	C	736	THR
1	C	761	GLN
1	D	40	ARG
1	D	41	LYS
1	D	51	ASN
1	D	73	GLU
1	D	90	LEU
1	D	110	ASP
1	D	145	GLU
1	D	160	VAL
1	D	170	ASN
1	D	207	VAL
1	D	246	LEU
1	D	253	ARG
1	D	254	VAL
1	D	272	ASN
1	D	276	LEU
1	D	303	VAL
1	D	326	ASP
1	D	332	GLU
1	D	336	ARG
1	D	385	CYS
1	D	392	LYS
1	D	436	LEU
1	D	440	THR
1	D	448	GLU
1	D	482	LEU
1	D	505	GLN
1	D	514	LEU
1	D	523	LYS
1	D	536	LYS
1	D	543	LEU
1	D	561	LEU
1	D	566	TYR
1	D	583	SER
1	D	603	VAL
1	D	658	ARG
1	D	679	ASN

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Mol	Chain	Res	Type
1	D	689	MET
1	D	701	LEU
1	D	702	LEU
1	D	736	THR
1	D	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	72	GLN
1	A	75	ASN
1	A	92	ASN
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	345	HIS
1	A	369	ASN
1	A	435	GLN
1	A	483	HIS
1	A	533	HIS
1	A	572	ASN
1	A	606	GLN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	761	GLN
1	B	51	ASN
1	B	72	GLN
1	B	75	ASN
1	B	92	ASN
1	B	169	ASN
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	345	HIS
1	B	369	ASN

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Mol	Chain	Res	Type
1	B	435	GLN
1	B	483	HIS
1	B	533	HIS
1	B	572	ASN
1	B	606	GLN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	731	GLN
1	B	761	GLN
1	C	51	ASN
1	C	169	ASN
1	C	170	ASN
1	C	247	GLN
1	C	272	ASN
1	C	314	GLN
1	C	369	ASN
1	C	377	ASN
1	C	388	GLN
1	C	483	HIS
1	C	487	ASN
1	C	533	HIS
1	C	572	ASN
1	C	612	GLN
1	C	679	ASN
1	C	694	ASN
1	C	704	HIS
1	C	718	GLN
1	C	761	GLN
1	D	51	ASN
1	D	123	GLN
1	D	169	ASN
1	D	170	ASN
1	D	272	ASN
1	D	314	GLN
1	D	369	ASN
1	D	377	ASN
1	D	388	GLN
1	D	483	HIS
1	D	487	ASN

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Mol	Chain	Res	Type
1	D	533	HIS
1	D	572	ASN
1	D	612	GLN
1	D	679	ASN
1	D	694	ASN
1	D	704	HIS
1	D	718	GLN
1	D	761	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](#)

1 ligand is 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	AAF	B	800	1	31,31,31	1.58	6 (19%)	37,42,42	1.03	2 (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
2	AAF	B	800	1	-	0/25/44/44	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	AAF	C14-N18	-5.07	1.34	1.47
2	B	800	AAF	C22-C21	2.09	1.42	1.38
2	B	800	AAF	C24-C23	2.29	1.43	1.39
2	B	800	AAF	C22-C23	2.44	1.43	1.39
2	B	800	AAF	C25-C20	2.85	1.44	1.39
2	B	800	AAF	C1-N8	3.20	1.41	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	AAF	C29-O28-C26	2.31	120.40	115.85
2	B	800	AAF	C12-C13-N8	2.66	107.36	103.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	AAF	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	726/726 (100%)	0.39	51 (7%)	17 17	16, 27, 56, 88	0
1	B	726/726 (100%)	0.42	65 (8%)	10 10	15, 28, 63, 85	0
1	C	726/726 (100%)	0.40	69 (9%)	9 9	18, 34, 61, 79	0
1	D	726/726 (100%)	0.35	58 (7%)	13 13	18, 32, 60, 79	0
All	All	2904/2904 (100%)	0.39	243 (8%)	12 12	15, 30, 60, 88	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	22.5
1	A	282	ALA	13.5
1	A	278	SER	11.9
1	C	39	SER	11.3
1	A	277	SER	10.9
1	A	280	THR	10.2
1	A	281	ASN	9.7
1	A	39	SER	9.6
1	B	73	GLU	8.4
1	D	39	SER	8.0
1	A	73	GLU	7.6
1	B	39	SER	7.6
1	C	333	SER	7.5
1	C	73	GLU	7.4
1	D	279	VAL	7.1
1	D	92	ASN	6.8
1	B	97	GLU	6.7
1	B	278	SER	6.6
1	A	276	LEU	6.5
1	A	40	ARG	6.3
1	C	138	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
1	D	73	GLU	5.9
1	D	278	SER	5.9
1	D	74	ASN	5.6
1	D	93	SER	5.6
1	B	279	VAL	5.5
1	A	333	SER	5.5
1	C	105	TYR	5.4
1	C	98	PHE	5.4
1	A	74	ASN	5.3
1	C	332	GLU	5.2
1	D	289	ALA	5.2
1	C	277	SER	5.1
1	B	277	SER	5.0
1	B	74	ASN	4.9
1	B	92	ASN	4.8
1	D	83	TYR	4.8
1	C	392	LYS	4.8
1	B	280	THR	4.8
1	C	40	ARG	4.7
1	A	342	ALA	4.7
1	D	342	ALA	4.6
1	B	71	LYS	4.5
1	B	341	VAL	4.5
1	D	277	SER	4.5
1	D	72	GLN	4.5
1	C	187	TRP	4.4
1	C	140	ARG	4.4
1	D	281	ASN	4.4
1	B	160	VAL	4.4
1	B	487	ASN	4.3
1	C	391	LYS	4.3
1	B	392	LYS	4.3
1	C	334	SER	4.2
1	B	40	ARG	4.2
1	B	138	ASN	4.2
1	D	71	LYS	4.2
1	D	99	GLY	4.2
1	A	72	GLN	4.2
1	C	71	LYS	4.2
1	D	412	SER	4.2
1	C	506	ASN	4.1
1	B	99	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	96	ASP	4.1
1	A	114	ILE	4.0
1	D	333	SER	4.0
1	D	334	SER	3.9
1	D	336	ARG	3.9
1	B	72	GLN	3.9
1	C	437	SER	3.9
1	A	366	LEU	3.9
1	A	521	GLU	3.9
1	B	105	TYR	3.9
1	B	63	ILE	3.8
1	C	390	ASP	3.8
1	D	90	LEU	3.8
1	B	134	ILE	3.8
1	B	139	LYS	3.8
1	D	391	LYS	3.8
1	B	333	SER	3.8
1	C	520	ASN	3.8
1	B	111	GLY	3.8
1	B	332	GLU	3.7
1	B	366	LEU	3.7
1	D	88	VAL	3.6
1	D	280	THR	3.6
1	C	96	ASP	3.5
1	D	97	GLU	3.5
1	B	101	SER	3.4
1	C	92	ASN	3.4
1	B	96	ASP	3.4
1	B	61	ARG	3.4
1	C	88	VAL	3.4
1	D	276	LEU	3.3
1	C	336	ARG	3.3
1	C	83	TYR	3.3
1	D	440	THR	3.2
1	D	487	ASN	3.2
1	B	289	ALA	3.2
1	C	74	ASN	3.2
1	D	91	GLU	3.2
1	A	92	ASN	3.2
1	C	389	ILE	3.2
1	B	489	LYS	3.2
1	A	506	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	289	ALA	3.1
1	B	282	ALA	3.1
1	D	332	GLU	3.1
1	C	289	ALA	3.1
1	B	66	HIS	3.1
1	D	486	VAL	3.1
1	C	440	THR	3.1
1	C	279	VAL	3.1
1	A	334	SER	3.1
1	B	342	ALA	3.0
1	B	336	ARG	3.0
1	B	502	LYS	3.0
1	A	145	GLU	3.0
1	C	99	GLY	2.9
1	C	161	GLY	2.9
1	A	98	PHE	2.9
1	A	412	SER	2.9
1	A	520	ASN	2.9
1	D	521	GLU	2.9
1	D	392	LYS	2.9
1	C	110	ASP	2.9
1	C	100	HIS	2.8
1	D	40	ARG	2.8
1	C	72	GLN	2.8
1	D	138	ASN	2.8
1	C	141	GLN	2.8
1	A	134	ILE	2.8
1	D	86	SER	2.8
1	C	505	GLN	2.8
1	A	93	SER	2.7
1	B	83	TYR	2.7
1	C	160	VAL	2.7
1	D	341	VAL	2.7
1	B	340	LEU	2.7
1	A	91	GLU	2.7
1	C	533	HIS	2.7
1	D	340	LEU	2.7
1	B	140	ARG	2.7
1	B	440	THR	2.7
1	B	330	TYR	2.6
1	A	90	LEU	2.6
1	B	334	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	520	ASN	2.6
1	C	442	VAL	2.6
1	A	71	LYS	2.6
1	A	83	TYR	2.6
1	B	764	SER	2.6
1	C	340	LEU	2.6
1	D	436	LEU	2.6
1	C	341	VAL	2.6
1	D	380	GLY	2.5
1	C	97	GLU	2.5
1	C	61	ARG	2.5
1	A	645	GLY	2.5
1	D	283	THR	2.5
1	A	336	ARG	2.5
1	D	100	HIS	2.5
1	C	90	LEU	2.5
1	A	140	ARG	2.5
1	C	147	ARG	2.5
1	D	489	LYS	2.5
1	C	366	LEU	2.4
1	A	160	VAL	2.4
1	A	764	SER	2.4
1	C	146	GLU	2.4
1	A	87	SER	2.4
1	C	441	LYS	2.4
1	D	505	GLN	2.4
1	B	147	ARG	2.4
1	B	442	VAL	2.4
1	C	91	GLU	2.4
1	C	137	LEU	2.4
1	D	160	VAL	2.3
1	B	137	LEU	2.3
1	D	147	ARG	2.3
1	D	520	ASN	2.3
1	A	102	ILE	2.3
1	A	505	GLN	2.3
1	B	54	ARG	2.3
1	C	276	LEU	2.3
1	A	97	GLU	2.3
1	D	101	SER	2.3
1	A	283	THR	2.3
1	D	61	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	68	TYR	2.3
1	B	276	LEU	2.3
1	C	93	SER	2.3
1	B	505	GLN	2.3
1	D	442	VAL	2.3
1	B	411	THR	2.3
1	C	502	LYS	2.3
1	C	521	GLU	2.3
1	D	452	GLU	2.2
1	A	99	GLY	2.2
1	C	114	ILE	2.2
1	B	144	THR	2.2
1	C	536	LYS	2.2
1	D	437	SER	2.2
1	B	60	LEU	2.2
1	B	75	ASN	2.2
1	C	338	ASN	2.2
1	A	187	TRP	2.2
1	B	412	SER	2.2
1	C	764	SER	2.2
1	C	82	GLU	2.2
1	C	87	SER	2.2
1	B	102	ILE	2.1
1	A	105	TYR	2.1
1	A	616	MET	2.1
1	B	141	GLN	2.1
1	C	384	ILE	2.1
1	B	115	LEU	2.1
1	C	393	ASP	2.1
1	C	101	SER	2.1
1	C	379	GLU	2.1
1	C	464	GLU	2.1
1	B	132	TYR	2.1
1	A	138	ASN	2.1
1	B	378	GLU	2.1
1	A	392	LYS	2.1
1	C	41	LYS	2.1
1	D	621	ASN	2.1
1	B	413	ASP	2.1
1	A	66	HIS	2.1
1	B	103	ASN	2.1
1	D	288	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	423	LYS	2.1
1	A	96	ASP	2.0
1	C	94	THR	2.0
1	C	342	ALA	2.0
1	B	222	PHE	2.0
1	A	622	LYS	2.0
1	D	66	HIS	2.0
1	A	393	ASP	2.0
1	C	281	ASN	2.0
1	D	676	PRO	2.0
1	B	90	LEU	2.0
1	D	465	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	AAF	B	800	29/29	0.89	0.16	2.82	26,31,48,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.