Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 07:31 AM EDT

PDB ID	:	2Q7R
Title	:	Crystal structure of human FLAP with an iodinated analog of MK-591
Authors	:	Ferguson, A.D.
Deposited on	:	2007-06-07
Resolution	:	4.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

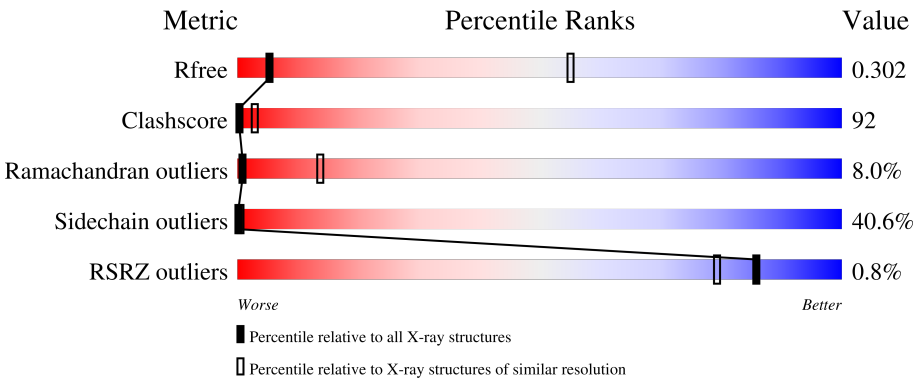
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 4.00 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}	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	161	%, 16%, 40%, 30%, •, 13%
1	B	161	11%, 42%, 34%, 5%, 8%
1	C	161	24%, 43%, 24%, •, 7%
1	D	161	%, 16%, 45%, 29%, •, 8%
1	E	161	%, 16%, 39%, 30%, •, 13%

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Mol	Chain	Length	Quality of chain
1	F	161	2% 13% 44% 33% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	3CS	A	503	-	-	X	-
2	3CS	C	501	-	-	X	-
2	3CS	D	505	-	-	X	-
2	3CS	E	506	-	-	X	-
2	3CS	F	504	-	-	X	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7254 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 Arachidonate 5-lipoxygenase-activating protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	140	1119	739	183	192	2	3	0	0	0
1	B	148	1186	782	192	207	2	3	0	0	0
1	C	149	1193	786	193	209	2	3	0	0	0
1	D	148	1186	782	192	207	2	3	0	0	0
1	E	140	1119	739	183	192	2	3	0	0	0
1	F	149	1193	786	193	209	2	3	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P20292
A	89	MSE	MET	modified residue	UNP P20292
A	125	MSE	MET	modified residue	UNP P20292
A	148	ALA	LYS	engineered mutation	UNP P20292
B	1	MSE	MET	modified residue	UNP P20292
B	89	MSE	MET	modified residue	UNP P20292
B	125	MSE	MET	modified residue	UNP P20292
B	148	ALA	LYS	engineered mutation	UNP P20292
C	1	MSE	MET	modified residue	UNP P20292
C	89	MSE	MET	modified residue	UNP P20292
C	125	MSE	MET	modified residue	UNP P20292
C	148	ALA	LYS	engineered mutation	UNP P20292
D	1	MSE	MET	modified residue	UNP P20292
D	89	MSE	MET	modified residue	UNP P20292
D	125	MSE	MET	modified residue	UNP P20292
D	148	ALA	LYS	engineered mutation	UNP P20292
E	1	MSE	MET	modified residue	UNP P20292

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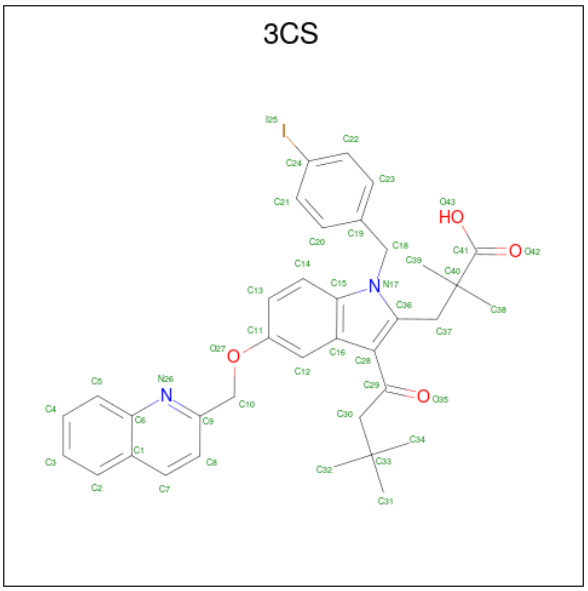
Chain	Residue	Modelled	Actual	Comment	Reference
E	89	MSE	MET	modified residue	UNP P20292
E	125	MSE	MET	modified residue	UNP P20292
E	148	ALA	LYS	engineered mutation	UNP P20292
F	1	MSE	MET	modified residue	UNP P20292
F	89	MSE	MET	modified residue	UNP P20292
F	125	MSE	MET	modified residue	UNP P20292
F	148	ALA	LYS	engineered mutation	UNP P20292

- Molecule 2 is 3-[3-(3,3-DIMETHYLBUTANOYL)-1-(4-IODOBENZYL)-5-(QUINOLIN-2-YLMETHOXY)-1H-INDOL-2-YL]-2,2-DIMETHYLPROPANOIC ACID (three-letter code: 3CS) (formula: $C_{36}H_{37}IN_2O_4$).



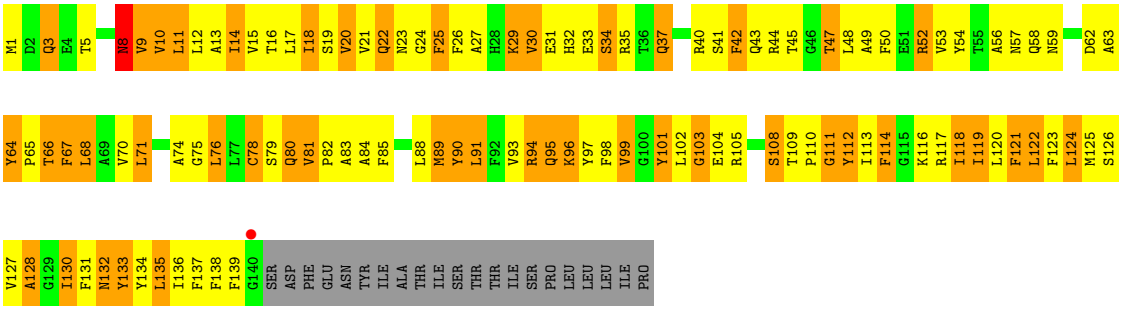
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	I	N	O	0	0
			43	36	1	2	4		
2	B	1	Total	C	I	N	O	0	0
			43	36	1	2	4		
2	C	1	Total	C	I	N	O	0	0
			43	36	1	2	4		
2	D	1	Total	C	I	N	O	0	0
			43	36	1	2	4		
2	E	1	Total	C	I	N	O	0	0
			43	36	1	2	4		
2	F	1	Total	C	I	N	O	0	0
			43	36	1	2	4		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

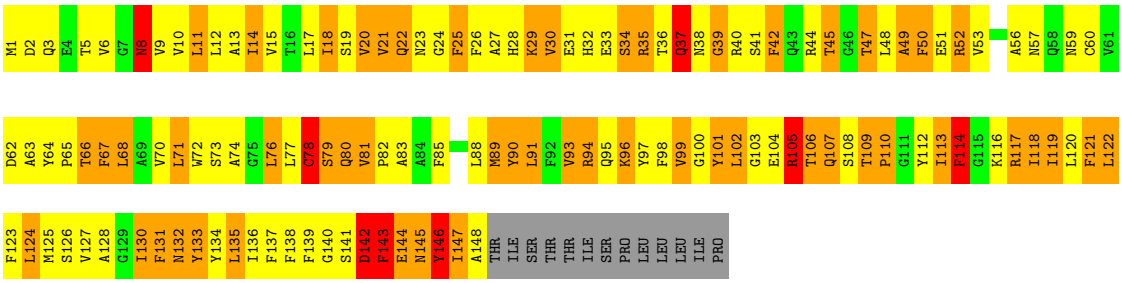
• Molecule 1: Arachidonate 5-lipoxygenase-activating protein

Chain A:



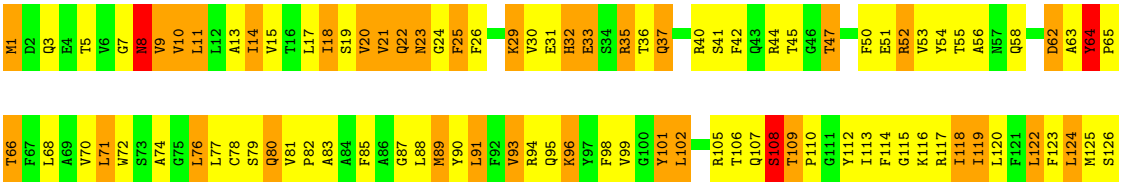
• Molecule 1: Arachidonate 5-lipoxygenase-activating protein

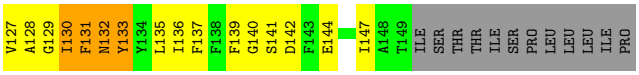
Chain B:



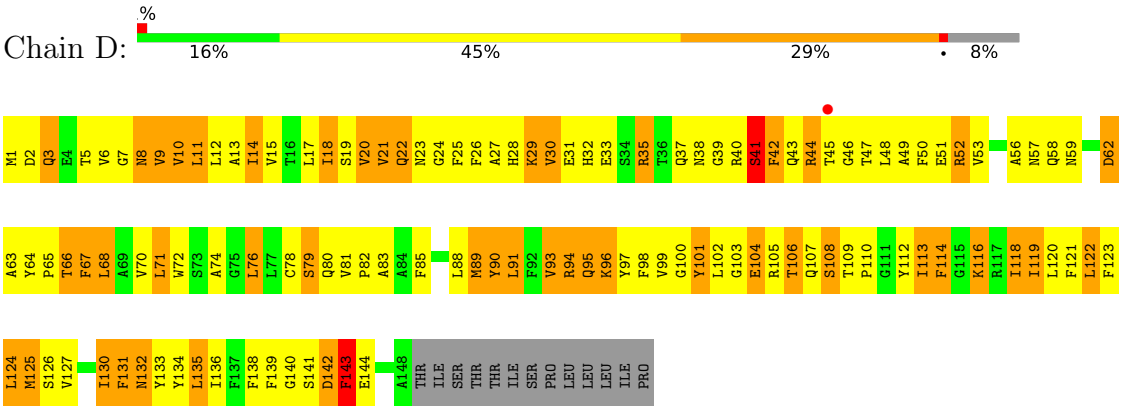
• Molecule 1: Arachidonate 5-lipoxygenase-activating protein

Chain C:

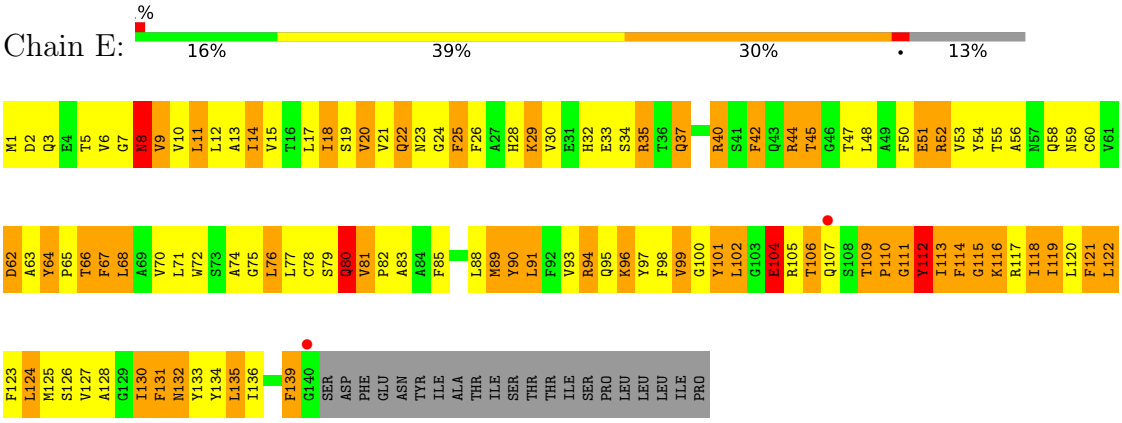




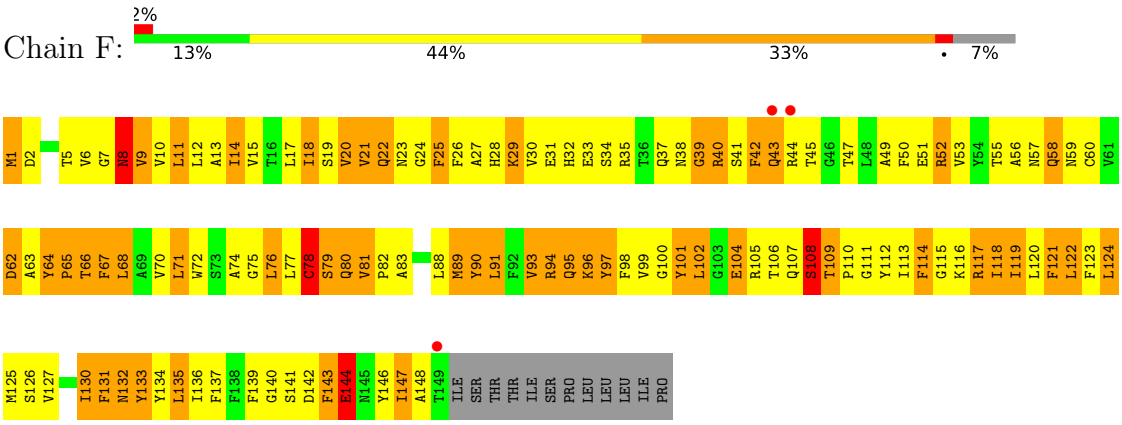
• Molecule 1: Arachidonate 5-lipoxygenase-activating protein



• Molecule 1: Arachidonate 5-lipoxygenase-activating protein



• Molecule 1: Arachidonate 5-lipoxygenase-activating protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	180.66Å 180.66Å 139.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.00 45.18 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-4.00) 99.5 (45.18-4.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 4.00Å)	Xtriage
Refinement program	BUSTER-TNT 1.9.3	Depositor
R, R_{free}	0.268 , 0.281 0.282 , 0.302	Depositor DCC
R_{free} test set	1021 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	135.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 92.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	7254	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.11% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3CS

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.37	0/1146	0.63	0/1550
1	B	0.35	0/1215	0.52	0/1644
1	C	0.39	0/1222	0.64	2/1654 (0.1%)
1	D	0.36	0/1215	0.54	0/1644
1	E	0.34	0/1146	0.59	2/1550 (0.1%)
1	F	0.40	0/1222	0.63	0/1654
All	All	0.37	0/7166	0.59	4/9696 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	109	THR	N-CA-C	7.89	132.30	111.00
1	E	109	THR	C-N-CD	-7.12	104.94	120.60
1	C	108	SER	N-CA-C	-6.82	92.60	111.00
1	E	104	GLU	N-CA-C	5.15	124.92	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1119	0	1116	234	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1186	0	1171	248	0
1	C	1193	0	1178	212	0
1	D	1186	0	1171	261	0
1	E	1119	0	1116	217	0
1	F	1193	0	1178	254	0
2	A	43	0	36	29	0
2	B	43	0	36	19	0
2	C	43	0	36	21	0
2	D	43	0	36	28	0
2	E	43	0	36	23	0
2	F	43	0	36	21	0
All	All	7254	0	7146	1321	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 92.

All (1321) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LEU:HD23	2:B:502:3CS:H302	1.21	1.18
1:F:81:VAL:HG13	1:F:82:PRO:HD3	1.22	1.17
1:F:74:ALA:HB1	1:F:125:MSE:HE2	1.19	1.16
1:F:120:LEU:HD23	2:F:504:3CS:H302	1.14	1.13
1:B:83:ALA:HB2	1:B:125:MSE:HE1	1.19	1.13
1:A:120:LEU:HD23	2:A:503:3CS:H302	1.29	1.11
1:C:11:LEU:H	1:C:11:LEU:HD22	1.12	1.10
1:F:119:ILE:HD11	2:F:504:3CS:H12	1.25	1.09
1:A:119:ILE:HD11	2:A:503:3CS:H12	1.32	1.09
1:F:53:VAL:HG23	1:F:102:LEU:HD21	1.35	1.08
1:D:74:ALA:HB1	1:D:125:MSE:HE2	1.30	1.07
1:F:83:ALA:HB2	1:F:125:MSE:HE1	1.35	1.06
1:F:94:ARG:HA	1:F:114:PHE:CZ	1.90	1.06
1:D:108:SER:HA	1:E:40:ARG:HD2	1.41	1.02
1:B:94:ARG:HG2	1:B:114:PHE:HE2	1.21	1.02
1:C:83:ALA:HB2	1:C:125:MSE:HE1	1.35	1.02
1:F:11:LEU:HD22	1:F:11:LEU:H	1.22	1.02
2:F:504:3CS:H301	2:F:504:3CS:H372	1.40	1.02
1:B:11:LEU:HD22	1:B:11:LEU:H	1.23	1.01
1:C:108:SER:O	1:C:110:PRO:HD2	1.59	1.01
1:B:124:LEU:HA	1:B:127:VAL:HG12	1.43	1.00
1:C:11:LEU:HD21	1:C:80:GLN:HE21	1.25	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ALA:HB2	1:A:125:MSE:HE1	1.44	0.99
1:E:52:ARG:HE	1:E:104:GLU:HB2	1.27	0.98
1:C:52:ARG:HB3	1:C:102:LEU:HB2	1.41	0.97
1:E:81:VAL:HG13	1:E:82:PRO:HD3	1.47	0.96
2:E:506:3CS:H323	2:E:506:3CS:H372	1.47	0.96
1:A:94:ARG:HG2	1:A:114:PHE:HE2	1.30	0.96
1:C:85:PHE:CZ	1:C:89:MSE:HE2	2.01	0.96
1:D:81:VAL:HG23	1:D:82:PRO:HD3	1.46	0.95
1:A:94:ARG:HG2	1:A:114:PHE:CE2	2.01	0.95
1:B:145:ASN:ND2	1:B:145:ASN:H	1.64	0.95
1:C:74:ALA:HB1	1:C:125:MSE:HE2	1.48	0.95
1:D:11:LEU:HD22	1:D:11:LEU:H	1.30	0.94
1:B:74:ALA:HB1	1:B:125:MSE:HE2	1.46	0.94
1:F:94:ARG:HA	1:F:114:PHE:CE2	2.03	0.94
1:B:81:VAL:HG13	1:B:82:PRO:HD3	1.51	0.93
1:D:20:VAL:HG22	1:F:66:THR:HG22	1.51	0.93
1:A:124:LEU:HA	1:A:127:VAL:HG12	1.51	0.92
1:C:52:ARG:HH21	1:C:105:ARG:HA	1.33	0.92
1:E:124:LEU:HA	1:E:127:VAL:HG12	1.49	0.92
1:E:120:LEU:HD22	2:E:506:3CS:H313	1.52	0.92
1:C:124:LEU:HA	1:C:127:VAL:HG12	1.50	0.92
1:D:45:THR:HB	1:F:44:ARG:HG3	1.50	0.92
1:D:43:GLN:HA	1:D:44:ARG:HH21	1.34	0.91
1:D:124:LEU:HA	1:D:127:VAL:HG12	1.50	0.91
1:B:83:ALA:HB2	1:B:125:MSE:CE	1.99	0.91
1:F:124:LEU:HA	1:F:127:VAL:HG12	1.53	0.90
1:B:79:SER:HB3	1:B:82:PRO:HG2	1.54	0.90
1:D:89:MSE:HB3	1:D:118:ILE:HD11	1.54	0.90
1:D:120:LEU:HD23	2:D:505:3CS:H301	1.51	0.90
1:B:94:ARG:HG2	1:B:114:PHE:CE2	2.08	0.89
1:E:83:ALA:HB2	1:E:125:MSE:HE1	1.52	0.89
1:A:21:VAL:HG22	2:C:501:3CS:H341	1.53	0.89
1:D:108:SER:CA	1:E:40:ARG:HD2	2.03	0.89
1:E:44:ARG:HH12	1:F:43:GLN:HB2	1.38	0.88
1:F:25:PHE:HE1	1:F:29:LYS:HG2	1.37	0.88
1:D:31:GLU:HG2	1:F:113:ILE:HD11	1.55	0.88
1:D:101:TYR:HA	1:D:109:THR:CG2	2.04	0.88
1:D:79:SER:HB3	1:D:82:PRO:HG2	1.54	0.87
1:B:70:VAL:HB	1:B:122:LEU:HB3	1.57	0.87
1:D:35:ARG:HE	1:D:35:ARG:HA	1.38	0.87
1:E:35:ARG:HA	1:E:35:ARG:HE	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ALA:HB2	1:D:125:MSE:HE1	1.57	0.87
1:A:52:ARG:NH2	1:A:108:SER:HB3	1.89	0.86
1:C:11:LEU:CD2	1:C:80:GLN:HE21	1.89	0.86
1:B:8:ASN:H	1:B:8:ASN:ND2	1.70	0.86
1:E:89:MSE:HB3	1:E:118:ILE:HD11	1.57	0.85
1:F:96:LYS:N	1:F:96:LYS:HD2	1.90	0.85
1:C:52:ARG:HB3	1:C:102:LEU:CB	2.05	0.85
1:F:120:LEU:HD23	2:F:504:3CS:C30	2.04	0.85
1:F:89:MSE:HB3	1:F:118:ILE:HD11	1.59	0.85
1:A:8:ASN:H	1:A:8:ASN:ND2	1.74	0.85
1:A:96:LYS:N	1:A:96:LYS:HD2	1.92	0.85
1:F:19:SER:HB3	1:F:91:LEU:HD11	1.57	0.85
1:E:11:LEU:H	1:E:11:LEU:HD22	1.40	0.85
1:E:53:VAL:CG2	1:E:102:LEU:HD23	2.07	0.85
1:A:120:LEU:HA	2:A:503:3CS:H313	1.56	0.84
1:B:96:LYS:HD2	1:B:96:LYS:N	1.92	0.84
1:A:42:PHE:HD2	1:A:50:PHE:HZ	1.21	0.84
1:E:44:ARG:NH1	1:F:43:GLN:HB2	1.91	0.84
1:F:119:ILE:HD11	2:F:504:3CS:C12	2.05	0.83
1:A:102:LEU:HG	1:A:103:GLY:H	1.42	0.83
1:C:96:LYS:HD2	1:C:96:LYS:N	1.92	0.83
1:D:96:LYS:HD2	1:D:96:LYS:N	1.91	0.83
1:B:120:LEU:HD23	2:B:502:3CS:C30	2.08	0.83
1:C:70:VAL:HB	1:C:122:LEU:HB3	1.60	0.82
1:B:144:GLU:HB3	1:B:146:TYR:CZ	2.15	0.82
1:A:89:MSE:HB3	1:A:118:ILE:HD11	1.59	0.82
1:F:53:VAL:CG2	1:F:102:LEU:HD21	2.09	0.82
1:A:44:ARG:HE	1:C:45:THR:HG21	1.43	0.82
1:D:94:ARG:HG2	1:D:114:PHE:CZ	2.15	0.82
1:B:8:ASN:ND2	1:B:8:ASN:N	2.28	0.82
1:A:20:VAL:HG22	1:C:66:THR:HG22	1.60	0.81
1:A:120:LEU:HD23	2:A:503:3CS:C30	2.08	0.81
1:A:119:ILE:HD11	2:A:503:3CS:C12	2.09	0.81
1:D:70:VAL:HB	1:D:122:LEU:HB3	1.61	0.81
2:B:502:3CS:H301	2:B:502:3CS:H372	1.61	0.81
1:B:90:TYR:HE1	1:B:94:ARG:HG3	1.45	0.80
1:B:124:LEU:HA	1:B:127:VAL:CG1	2.11	0.80
1:A:31:GLU:HG2	1:C:113:ILE:HD11	1.63	0.80
1:A:123:PHE:HD1	1:A:124:LEU:HD13	1.46	0.80
1:B:101:TYR:OH	1:C:42:PHE:HB3	1.81	0.80
1:E:116:LYS:HA	1:E:119:ILE:CD1	2.10	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:HE	1:B:103:GLY:HA2	1.46	0.80
2:E:506:3CS:H341	1:F:21:VAL:HG22	1.62	0.80
1:C:30:VAL:HG22	1:C:53:VAL:HG12	1.64	0.80
1:C:139:PHE:HA	1:C:142:ASP:OD2	1.82	0.80
1:A:116:LYS:HE3	2:A:503:3CS:H391	1.63	0.79
1:B:34:SER:O	1:B:39:GLY:HA3	1.81	0.79
1:C:85:PHE:HZ	1:C:89:MSE:HE2	1.43	0.79
1:E:101:TYR:OH	1:F:40:ARG:HG2	1.83	0.78
1:F:83:ALA:HB2	1:F:125:MSE:CE	2.11	0.78
1:E:96:LYS:HD2	1:E:96:LYS:N	1.97	0.78
1:F:133:TYR:HE1	1:F:137:PHE:HB2	1.47	0.78
1:A:40:ARG:CB	1:C:52:ARG:HH12	1.97	0.78
1:F:81:VAL:CG1	1:F:82:PRO:HD3	2.09	0.78
1:A:108:SER:O	1:A:110:PRO:HD3	1.84	0.77
1:C:124:LEU:HA	1:C:127:VAL:CG1	2.14	0.77
1:B:145:ASN:H	1:B:145:ASN:HD22	1.27	0.77
1:D:81:VAL:CG2	1:D:82:PRO:HD3	2.14	0.77
1:D:116:LYS:HA	1:D:116:LYS:HZ3	1.48	0.77
1:F:72:TRP:O	1:F:76:LEU:HD22	1.83	0.77
1:D:44:ARG:N	1:D:44:ARG:HE	1.82	0.77
1:B:89:MSE:HB3	1:B:118:ILE:HD11	1.66	0.77
1:C:52:ARG:CB	1:C:102:LEU:HB2	2.15	0.77
1:F:8:ASN:H	1:F:8:ASN:ND2	1.82	0.77
1:B:120:LEU:HA	2:B:502:3CS:H313	1.65	0.76
1:A:70:VAL:HB	1:A:122:LEU:HB3	1.68	0.76
1:F:43:GLN:O	1:F:45:THR:HG23	1.86	0.76
1:F:74:ALA:HB1	1:F:125:MSE:CE	2.10	0.76
1:D:66:THR:HG22	1:E:20:VAL:HG22	1.67	0.76
1:E:124:LEU:HA	1:E:127:VAL:CG1	2.15	0.76
1:C:119:ILE:HD11	2:C:501:3CS:H12	1.66	0.76
1:A:11:LEU:HD23	1:A:80:GLN:HG2	1.67	0.76
1:D:44:ARG:HB3	1:E:44:ARG:NH2	2.01	0.76
1:A:8:ASN:ND2	1:A:8:ASN:N	2.30	0.75
1:A:34:SER:HB2	1:A:42:PHE:HE2	1.50	0.75
1:A:110:PRO:HB3	1:B:42:PHE:H	1.51	0.75
1:D:101:TYR:HA	1:D:109:THR:HG23	1.69	0.75
1:B:8:ASN:N	1:B:8:ASN:HD22	1.82	0.75
1:A:78:CYS:HB3	1:A:125:MSE:HE3	1.68	0.75
1:D:74:ALA:CB	1:D:125:MSE:HE2	2.14	0.75
1:B:19:SER:HB3	1:B:91:LEU:HD11	1.67	0.74
1:E:30:VAL:HG22	1:E:53:VAL:HG12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:LEU:HD23	1:B:80:GLN:NE2	2.02	0.74
1:C:63:ALA:HB2	1:C:114:PHE:CE2	2.23	0.74
1:E:120:LEU:CD2	2:E:506:3CS:H313	2.16	0.74
1:A:85:PHE:HZ	1:A:89:MSE:HE2	1.51	0.74
1:D:116:LYS:HE3	2:D:505:3CS:C15	2.18	0.74
1:A:19:SER:HB3	1:A:91:LEU:HD11	1.69	0.74
1:A:83:ALA:HB2	1:A:125:MSE:CE	2.16	0.74
1:D:105:ARG:O	1:D:107:GLN:N	2.21	0.74
1:F:74:ALA:CB	1:F:125:MSE:HE2	2.11	0.74
1:A:85:PHE:CZ	1:A:89:MSE:HE2	2.23	0.74
2:C:501:3CS:H23	2:C:501:3CS:O42	1.88	0.74
1:C:11:LEU:HD22	1:C:11:LEU:N	1.95	0.74
1:C:89:MSE:HB3	1:C:118:ILE:HD11	1.69	0.74
1:E:66:THR:HG22	1:F:20:VAL:HG22	1.67	0.74
1:E:70:VAL:HB	1:E:122:LEU:HB3	1.69	0.74
1:B:33:GLU:HG3	1:B:49:ALA:O	1.88	0.73
1:B:26:PHE:HA	1:B:98:PHE:HE2	1.53	0.73
1:A:42:PHE:HD2	1:A:50:PHE:CZ	2.05	0.73
1:E:53:VAL:HG22	1:E:102:LEU:HD23	1.70	0.73
1:A:8:ASN:N	1:A:8:ASN:HD22	1.83	0.73
1:E:116:LYS:HA	1:E:119:ILE:HD11	1.68	0.73
1:A:120:LEU:HD13	1:A:124:LEU:CD2	2.18	0.73
1:A:120:LEU:CD2	2:A:503:3CS:H302	2.14	0.73
1:B:11:LEU:HD23	1:B:80:GLN:HE22	1.53	0.73
1:B:83:ALA:CB	1:B:125:MSE:HE1	2.11	0.73
1:D:120:LEU:HD23	2:D:505:3CS:C30	2.19	0.73
1:C:120:LEU:HD13	1:C:124:LEU:CD2	2.19	0.73
1:F:94:ARG:HA	1:F:114:PHE:HZ	1.48	0.73
1:A:44:ARG:NE	1:C:45:THR:HG21	2.04	0.73
1:D:19:SER:HB3	1:D:91:LEU:HD11	1.70	0.73
1:C:10:VAL:HG13	1:C:14:ILE:CD1	2.19	0.72
1:A:44:ARG:HE	1:C:45:THR:CG2	2.01	0.72
1:C:8:ASN:ND2	1:C:8:ASN:H	1.86	0.72
1:D:20:VAL:HG22	1:F:66:THR:CG2	2.19	0.72
1:A:43:GLN:HE22	1:C:54:TYR:HB3	1.55	0.72
2:A:503:3CS:H382	2:A:503:3CS:H23	1.71	0.72
1:C:19:SER:HB3	1:C:91:LEU:HD11	1.70	0.72
1:D:116:LYS:HZ1	2:D:505:3CS:C16	2.03	0.72
1:F:17:LEU:O	1:F:20:VAL:HG12	1.89	0.72
1:A:21:VAL:CG2	2:C:501:3CS:H341	2.20	0.72
2:D:505:3CS:C23	2:D:505:3CS:H371	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:PHE:CD1	1:F:43:GLN:N	2.58	0.72
1:E:83:ALA:HB2	1:E:125:MSE:CE	2.18	0.72
1:D:124:LEU:HA	1:D:127:VAL:CG1	2.20	0.72
1:E:48:LEU:HD11	1:E:52:ARG:HD2	1.72	0.72
1:E:67:PHE:HB2	1:E:90:TYR:HE2	1.54	0.72
1:D:45:THR:CB	1:F:44:ARG:HG3	2.19	0.72
1:A:66:THR:HG22	1:B:20:VAL:HG22	1.72	0.72
1:B:26:PHE:HA	1:B:98:PHE:CE2	2.25	0.72
1:D:100:GLY:O	1:D:109:THR:HG23	1.90	0.72
1:D:43:GLN:CA	1:D:44:ARG:HH21	2.01	0.71
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.54	0.71
1:B:124:LEU:CA	1:B:127:VAL:HG12	2.18	0.71
1:E:97:TYR:HD2	1:E:114:PHE:CD2	2.08	0.71
1:B:66:THR:HG22	1:C:20:VAL:HG22	1.72	0.71
1:C:45:THR:HG23	1:C:51:GLU:OE2	1.89	0.71
1:E:8:ASN:ND2	1:E:8:ASN:H	1.86	0.71
1:C:14:ILE:O	1:C:18:ILE:HD12	1.89	0.71
1:D:27:ALA:HB2	2:F:504:3CS:C4	2.20	0.71
1:D:112:TYR:CE2	1:E:30:VAL:HG11	2.24	0.71
1:E:106:THR:HG22	1:E:107:GLN:HG3	1.71	0.71
1:B:120:LEU:CD2	2:B:502:3CS:H302	2.13	0.70
1:C:35:ARG:HE	1:C:35:ARG:HA	1.55	0.70
1:F:8:ASN:ND2	1:F:8:ASN:N	2.37	0.70
1:A:40:ARG:HB3	1:C:52:ARG:HH12	1.56	0.70
1:D:45:THR:HG22	1:D:46:GLY:H	1.55	0.70
1:F:11:LEU:HD23	1:F:80:GLN:NE2	2.07	0.70
1:F:107:GLN:O	1:F:108:SER:HB2	1.90	0.70
1:A:102:LEU:HG	1:A:103:GLY:N	2.05	0.70
1:C:90:TYR:HB2	1:C:118:ILE:HG21	1.72	0.70
1:D:94:ARG:HA	1:D:114:PHE:HE1	1.55	0.70
1:E:119:ILE:HD11	2:E:506:3CS:H12	1.74	0.70
1:A:67:PHE:HB2	1:A:90:TYR:HE2	1.57	0.70
1:F:11:LEU:H	1:F:11:LEU:CD2	2.01	0.70
1:D:8:ASN:N	1:D:8:ASN:ND2	2.38	0.69
1:D:10:VAL:HG13	1:D:14:ILE:HD12	1.74	0.69
1:E:52:ARG:HE	1:E:104:GLU:CB	2.05	0.69
1:F:26:PHE:HA	1:F:98:PHE:CE2	2.28	0.69
1:B:79:SER:HB3	1:B:82:PRO:CG	2.21	0.69
1:B:90:TYR:CE1	1:B:94:ARG:HG3	2.26	0.69
1:F:79:SER:OG	1:F:80:GLN:N	2.26	0.69
1:B:38:ASN:O	1:B:40:ARG:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ALA:CB	1:C:125:MSE:HE1	2.18	0.69
1:F:11:LEU:CD2	1:F:80:GLN:HE22	2.04	0.69
1:A:14:ILE:O	1:A:18:ILE:HD12	1.92	0.69
1:A:120:LEU:O	1:A:124:LEU:HD22	1.93	0.69
1:C:37:GLN:HA	1:C:37:GLN:OE1	1.91	0.69
1:C:52:ARG:NH2	1:C:105:ARG:HA	2.07	0.69
1:C:116:LYS:HG3	1:C:117:ARG:N	2.08	0.69
1:C:124:LEU:CA	1:C:127:VAL:HG12	2.21	0.69
1:D:101:TYR:CD1	1:D:109:THR:HG22	2.28	0.69
1:E:13:ALA:O	1:E:17:LEU:HD23	1.92	0.69
1:D:8:ASN:ND2	1:D:8:ASN:H	1.89	0.69
1:F:11:LEU:HD23	1:F:80:GLN:HE22	1.58	0.69
1:F:133:TYR:CE1	1:F:137:PHE:HB2	2.28	0.69
1:C:119:ILE:HD11	2:C:501:3CS:C12	2.23	0.68
1:A:30:VAL:CG2	1:A:53:VAL:HG12	2.24	0.68
1:E:120:LEU:HD13	1:E:124:LEU:CD2	2.23	0.68
1:E:42:PHE:HD1	1:E:42:PHE:H	1.41	0.68
1:B:30:VAL:HG22	1:B:53:VAL:HG12	1.75	0.68
1:F:39:GLY:O	1:F:41:SER:N	2.25	0.68
1:B:144:GLU:HB3	1:B:146:TYR:CE1	2.28	0.68
1:A:101:TYR:OH	1:B:42:PHE:HB3	1.93	0.68
1:D:45:THR:HG22	1:D:46:GLY:N	2.09	0.68
1:B:132:ASN:ND2	1:B:136:ILE:HD11	2.09	0.68
1:D:79:SER:HB3	1:D:82:PRO:CG	2.23	0.68
1:D:120:LEU:HD23	2:D:505:3CS:O35	1.94	0.68
1:D:11:LEU:HD22	1:D:11:LEU:N	2.06	0.67
1:E:114:PHE:HD1	1:E:114:PHE:N	1.92	0.67
1:F:96:LYS:HD2	1:F:96:LYS:H	1.56	0.67
1:D:124:LEU:CA	1:D:127:VAL:HG12	2.24	0.67
1:E:81:VAL:HG13	1:E:82:PRO:CD	2.23	0.67
1:E:102:LEU:HD22	1:E:102:LEU:O	1.94	0.67
1:A:26:PHE:HA	1:A:98:PHE:CE2	2.30	0.67
1:A:133:TYR:HA	1:A:136:ILE:HD12	1.76	0.67
1:D:10:VAL:HG13	1:D:14:ILE:CD1	2.25	0.67
1:C:8:ASN:ND2	1:C:8:ASN:N	2.42	0.67
1:C:120:LEU:O	1:C:124:LEU:HD22	1.95	0.67
1:D:13:ALA:O	1:D:17:LEU:HD23	1.94	0.67
1:B:89:MSE:O	1:B:93:VAL:HG23	1.95	0.67
1:A:11:LEU:HD22	1:A:80:GLN:NE2	2.09	0.67
1:A:14:ILE:HG22	1:A:15:VAL:N	2.10	0.67
1:B:71:LEU:HD22	1:B:71:LEU:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:HIS:O	1:C:36:THR:HG23	1.95	0.67
1:D:79:SER:CB	1:D:82:PRO:HG2	2.25	0.67
1:F:23:ASN:OD1	1:F:94:ARG:NH2	2.27	0.67
1:A:10:VAL:HG13	1:A:14:ILE:CD1	2.23	0.67
1:A:103:GLY:O	1:A:104:GLU:HG3	1.95	0.67
1:B:11:LEU:CD2	1:B:80:GLN:HE22	2.07	0.67
1:B:17:LEU:O	1:B:20:VAL:HG12	1.95	0.66
1:F:6:VAL:O	1:F:10:VAL:HG23	1.96	0.66
1:F:25:PHE:CE1	1:F:29:LYS:HG2	2.26	0.66
1:F:52:ARG:HG3	1:F:52:ARG:HH11	1.60	0.66
1:D:42:PHE:HE2	1:F:112:TYR:HA	1.58	0.66
1:D:35:ARG:HA	1:D:35:ARG:NE	2.11	0.66
1:B:117:ARG:HH12	1:F:141:SER:CB	2.08	0.66
1:F:104:GLU:O	1:F:105:ARG:HG2	1.94	0.66
2:A:503:3CS:H382	2:A:503:3CS:H182	1.76	0.66
1:B:35:ARG:O	1:B:37:GLN:N	2.28	0.66
1:C:11:LEU:HD21	1:C:80:GLN:NE2	2.06	0.66
1:E:8:ASN:ND2	1:E:8:ASN:N	2.42	0.66
1:B:141:SER:OG	1:B:142:ASP:N	2.29	0.66
1:A:124:LEU:CA	1:A:127:VAL:HG12	2.26	0.66
1:F:126:SER:O	1:F:130:ILE:HB	1.96	0.66
1:A:34:SER:CB	1:A:42:PHE:HE2	2.09	0.65
1:D:42:PHE:CE2	1:F:112:TYR:HA	2.31	0.65
1:E:35:ARG:HA	1:E:35:ARG:NE	2.11	0.65
1:A:124:LEU:HA	1:A:127:VAL:CG1	2.24	0.65
1:C:18:ILE:CG2	1:C:91:LEU:HD23	2.25	0.65
1:C:25:PHE:HE1	1:C:29:LYS:HG2	1.62	0.65
1:D:44:ARG:NH1	1:F:51:GLU:HG2	2.11	0.65
1:D:110:PRO:HG3	1:E:40:ARG:HD3	1.78	0.65
1:F:120:LEU:CD2	2:F:504:3CS:H302	2.08	0.65
1:F:124:LEU:HA	1:F:127:VAL:CG1	2.25	0.65
1:A:99:VAL:O	1:A:102:LEU:HB3	1.96	0.65
1:B:112:TYR:CD2	1:C:30:VAL:HG11	2.31	0.65
1:B:132:ASN:HD21	1:B:136:ILE:HD11	1.60	0.65
2:A:503:3CS:H23	2:A:503:3CS:C38	2.27	0.65
1:B:44:ARG:O	1:B:45:THR:HB	1.95	0.65
1:D:11:LEU:HD23	1:D:80:GLN:NE2	2.10	0.65
1:E:81:VAL:CG1	1:E:82:PRO:HD3	2.24	0.65
1:F:26:PHE:HA	1:F:98:PHE:HE2	1.60	0.65
1:F:120:LEU:HD13	1:F:124:LEU:HD22	1.77	0.65
1:F:124:LEU:CA	1:F:127:VAL:HG12	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:SER:HB2	1:A:42:PHE:CE2	2.29	0.65
2:C:501:3CS:H371	2:C:501:3CS:C23	2.27	0.65
1:D:30:VAL:HG22	1:D:53:VAL:HG12	1.78	0.65
1:E:37:GLN:HE21	1:E:37:GLN:HA	1.61	0.65
1:C:11:LEU:HD23	1:C:80:GLN:CG	2.27	0.65
1:A:42:PHE:CE1	1:C:112:TYR:HE1	2.15	0.64
1:E:124:LEU:CA	1:E:127:VAL:HG12	2.22	0.64
1:E:125:MSE:O	1:E:128:ALA:HB3	1.97	0.64
1:D:120:LEU:CD2	2:D:505:3CS:H322	2.27	0.64
1:E:14:ILE:O	1:E:18:ILE:HD12	1.98	0.64
2:F:504:3CS:H23	2:F:504:3CS:O43	1.98	0.64
1:A:30:VAL:HG22	1:A:53:VAL:HG12	1.78	0.64
1:D:11:LEU:H	1:D:11:LEU:CD2	2.07	0.64
1:D:23:ASN:OD1	1:D:94:ARG:NH2	2.31	0.64
1:E:19:SER:HB3	1:E:91:LEU:HD11	1.78	0.64
1:A:26:PHE:HA	1:A:98:PHE:HE2	1.60	0.64
1:A:42:PHE:CD1	1:A:42:PHE:N	2.65	0.64
2:B:502:3CS:H182	2:B:502:3CS:O42	1.97	0.64
1:F:119:ILE:CD1	2:F:504:3CS:H12	2.16	0.64
1:F:142:ASP:C	1:F:144:GLU:H	2.00	0.64
1:A:40:ARG:HB2	1:C:52:ARG:HH12	1.63	0.63
1:A:74:ALA:HB2	1:A:122:LEU:O	1.98	0.63
1:A:64:TYR:CZ	1:A:68:LEU:HD21	2.33	0.63
1:A:10:VAL:HG21	1:C:133:TYR:CD2	2.33	0.63
1:B:6:VAL:O	1:B:10:VAL:HG23	1.99	0.63
1:B:11:LEU:HD23	1:B:80:GLN:OE1	1.98	0.63
1:D:33:GLU:HB3	1:D:50:PHE:HB2	1.80	0.63
1:B:10:VAL:HG12	1:B:11:LEU:HD13	1.79	0.63
1:E:52:ARG:HG3	1:E:52:ARG:HH11	1.64	0.63
2:E:506:3CS:H341	1:F:21:VAL:CG2	2.29	0.63
1:D:40:ARG:HB3	1:F:105:ARG:HH11	1.62	0.63
1:A:42:PHE:CD1	1:C:112:TYR:HE1	2.16	0.63
1:D:10:VAL:HG21	1:F:133:TYR:CD2	2.33	0.63
1:D:62:ASP:HB2	2:D:505:3CS:H2	1.81	0.63
1:E:97:TYR:HE2	1:E:114:PHE:CE1	2.17	0.63
1:C:11:LEU:H	1:C:11:LEU:CD2	1.96	0.63
1:C:125:MSE:O	1:C:128:ALA:HB3	1.97	0.63
1:D:133:TYR:HA	1:D:136:ILE:HD12	1.79	0.63
1:A:120:LEU:HD13	1:A:124:LEU:HD21	1.81	0.62
1:D:56:ALA:HA	1:D:101:TYR:CD2	2.34	0.62
1:E:10:VAL:HG13	1:E:14:ILE:CD1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:120:LEU:O	1:E:124:LEU:HD22	1.98	0.62
1:F:97:TYR:C	1:F:97:TYR:HD1	2.02	0.62
1:A:42:PHE:CD2	1:A:50:PHE:HZ	2.11	0.62
1:E:37:GLN:HE21	1:E:37:GLN:CA	2.11	0.62
1:E:116:LYS:HA	1:E:119:ILE:HD13	1.79	0.62
1:D:116:LYS:HZ1	2:D:505:3CS:C12	2.12	0.62
1:F:97:TYR:C	1:F:97:TYR:CD1	2.72	0.62
1:A:94:ARG:HA	1:A:114:PHE:HE2	1.63	0.62
1:A:123:PHE:HD1	1:A:124:LEU:CD1	2.12	0.62
1:B:120:LEU:O	1:B:124:LEU:HD22	1.99	0.62
1:E:26:PHE:HA	1:E:98:PHE:HE2	1.64	0.62
2:E:506:3CS:C4	1:F:27:ALA:HB2	2.30	0.62
1:D:72:TRP:O	1:D:76:LEU:HD22	1.99	0.62
1:D:120:LEU:HD13	1:D:124:LEU:CD2	2.29	0.62
1:E:26:PHE:HA	1:E:98:PHE:CE2	2.34	0.62
1:F:11:LEU:HD22	1:F:11:LEU:N	2.04	0.62
1:E:89:MSE:O	1:E:93:VAL:HG23	2.00	0.62
1:A:116:LYS:HE3	2:A:503:3CS:C39	2.29	0.62
1:B:120:LEU:HD13	1:B:124:LEU:CD2	2.30	0.62
1:C:126:SER:O	1:C:130:ILE:HB	2.00	0.62
1:D:42:PHE:N	1:D:42:PHE:CD1	2.67	0.62
1:E:11:LEU:HD23	1:E:80:GLN:CD	2.21	0.62
1:F:67:PHE:HB2	1:F:90:TYR:HE2	1.65	0.62
1:A:110:PRO:HB3	1:B:42:PHE:N	2.14	0.61
1:D:103:GLY:O	1:D:104:GLU:HG3	2.00	0.61
1:A:111:GLY:HA2	1:B:31:GLU:OE2	2.00	0.61
1:D:120:LEU:HD13	1:D:124:LEU:HD22	1.81	0.61
1:C:106:THR:HG22	1:C:107:GLN:N	2.14	0.61
1:D:24:GLY:C	2:F:504:3CS:H20	2.21	0.61
1:C:30:VAL:HA	1:C:53:VAL:HG11	1.83	0.61
1:F:67:PHE:CG	1:F:90:TYR:CE2	2.89	0.61
1:A:116:LYS:CE	2:A:503:3CS:H391	2.30	0.61
1:C:81:VAL:HB	1:C:82:PRO:HD3	1.83	0.61
1:C:119:ILE:CD1	2:C:501:3CS:H12	2.31	0.61
1:B:142:ASP:O	1:B:144:GLU:N	2.33	0.61
1:C:78:CYS:O	1:C:125:MSE:HE3	2.00	0.61
2:C:501:3CS:H371	2:C:501:3CS:C19	2.30	0.61
1:E:114:PHE:N	1:E:114:PHE:CD1	2.64	0.61
1:F:95:GLN:OE1	1:F:95:GLN:HA	2.01	0.61
1:F:121:PHE:CE1	1:F:125:MSE:HG3	2.36	0.61
1:B:123:PHE:CE2	1:C:21:VAL:HG23	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:LEU:HD23	1:E:80:GLN:OE1	2.01	0.60
1:B:90:TYR:CA	1:B:118:ILE:HD13	2.32	0.60
1:C:10:VAL:O	1:C:14:ILE:HD12	2.01	0.60
1:D:96:LYS:HD2	1:D:96:LYS:H	1.67	0.60
1:F:40:ARG:HG3	1:F:40:ARG:O	2.01	0.60
1:B:120:LEU:HD13	1:B:124:LEU:HD22	1.82	0.60
1:B:136:ILE:HA	1:B:140:GLY:HA3	1.82	0.60
1:B:145:ASN:O	1:B:147:ILE:N	2.29	0.60
1:E:45:THR:HG22	1:F:43:GLN:HG3	1.83	0.60
1:F:89:MSE:O	1:F:93:VAL:HG23	2.01	0.60
1:A:97:TYR:HD2	1:A:114:PHE:CD2	2.19	0.60
1:C:30:VAL:HG22	1:C:53:VAL:CG1	2.30	0.60
2:D:505:3CS:H20	1:E:24:GLY:C	2.22	0.60
1:B:23:ASN:OD1	1:B:94:ARG:NH2	2.34	0.60
1:E:126:SER:O	1:E:130:ILE:HB	2.02	0.60
1:B:11:LEU:O	1:B:15:VAL:HG12	2.02	0.60
1:C:120:LEU:HD13	1:C:124:LEU:HD22	1.82	0.60
1:F:133:TYR:CD1	1:F:133:TYR:C	2.74	0.60
1:A:94:ARG:HA	1:A:114:PHE:CE2	2.37	0.60
1:B:95:GLN:OE1	1:B:95:GLN:HA	2.00	0.60
1:D:40:ARG:HB3	1:F:105:ARG:NH1	2.16	0.60
1:B:145:ASN:ND2	1:B:145:ASN:N	2.39	0.60
1:C:120:LEU:HD23	2:C:501:3CS:O35	2.01	0.60
1:D:81:VAL:HG23	1:D:82:PRO:CD	2.27	0.60
1:E:120:LEU:HD13	1:E:124:LEU:HD22	1.82	0.60
1:B:11:LEU:HD23	1:B:80:GLN:CD	2.22	0.60
1:B:109:THR:N	1:B:110:PRO:HD3	2.17	0.60
1:D:95:GLN:OE1	1:D:95:GLN:HA	2.01	0.60
1:F:140:GLY:C	1:F:142:ASP:H	2.05	0.60
1:A:10:VAL:HG12	1:A:11:LEU:HD13	1.82	0.60
1:A:119:ILE:CD1	2:A:503:3CS:H12	2.20	0.60
2:B:502:3CS:C23	2:B:502:3CS:H371	2.32	0.60
1:F:8:ASN:N	1:F:8:ASN:HD22	1.98	0.60
1:F:39:GLY:C	1:F:41:SER:H	2.05	0.59
1:F:67:PHE:O	1:F:70:VAL:HG22	2.02	0.59
1:D:14:ILE:O	1:D:18:ILE:HD12	2.02	0.59
1:E:90:TYR:HB2	1:E:118:ILE:HG21	1.83	0.59
1:F:37:GLN:HG3	1:F:47:THR:OG1	2.02	0.59
2:D:505:3CS:H341	1:E:21:VAL:HA	1.85	0.59
1:E:48:LEU:HD11	1:E:52:ARG:CD	2.31	0.59
1:B:11:LEU:H	1:B:11:LEU:CD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ARG:NE	1:B:103:GLY:HA2	2.17	0.59
1:D:126:SER:O	1:D:130:ILE:HB	2.01	0.59
1:A:113:ILE:HD12	1:B:31:GLU:HG2	1.84	0.59
1:B:30:VAL:CG2	1:B:53:VAL:HG12	2.32	0.59
1:B:64:TYR:CZ	1:B:68:LEU:HD21	2.37	0.59
1:C:33:GLU:HG3	1:C:50:PHE:HA	1.85	0.59
1:D:44:ARG:NH1	1:F:55:THR:OG1	2.36	0.59
2:A:503:3CS:C19	2:A:503:3CS:H371	2.32	0.59
1:C:114:PHE:HD1	1:C:115:GLY:N	2.01	0.59
1:E:85:PHE:HZ	1:E:89:MSE:HE2	1.66	0.59
1:E:132:ASN:HD21	1:E:136:ILE:HD11	1.68	0.59
1:F:21:VAL:HG12	1:F:22:GLN:N	2.16	0.59
1:D:35:ARG:NH2	1:D:39:GLY:HA2	2.18	0.59
1:F:120:LEU:CD2	2:F:504:3CS:H313	2.33	0.59
1:A:54:TYR:HD2	1:B:44:ARG:HH12	1.47	0.59
1:D:41:SER:HA	1:F:110:PRO:HD2	1.83	0.59
1:E:97:TYR:OH	1:E:111:GLY:HA2	2.03	0.59
1:F:56:ALA:HA	1:F:101:TYR:CD2	2.36	0.59
2:D:505:3CS:H371	2:D:505:3CS:C19	2.33	0.59
1:E:11:LEU:HD23	1:E:80:GLN:NE2	2.18	0.59
1:E:85:PHE:CZ	1:E:89:MSE:HE2	2.38	0.59
1:E:139:PHE:CD1	1:E:139:PHE:N	2.69	0.59
1:B:13:ALA:O	1:B:17:LEU:HD23	2.03	0.59
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.68	0.59
1:D:39:GLY:O	1:F:109:THR:HB	2.01	0.59
1:D:94:ARG:HA	1:D:114:PHE:CE1	2.38	0.59
1:F:10:VAL:HG13	1:F:14:ILE:CD1	2.33	0.59
1:B:44:ARG:CZ	1:C:44:ARG:HH22	2.15	0.58
1:D:43:GLN:HA	1:D:44:ARG:NH2	2.14	0.58
1:E:42:PHE:N	1:E:42:PHE:CD1	2.71	0.58
1:C:85:PHE:CE1	1:C:89:MSE:HG2	2.38	0.58
1:A:10:VAL:HG21	1:C:133:TYR:CE2	2.38	0.58
1:B:121:PHE:CE1	1:B:125:MSE:HG3	2.38	0.58
1:C:56:ALA:HA	1:C:101:TYR:HD2	1.66	0.58
1:D:108:SER:HA	1:E:40:ARG:CD	2.25	0.58
1:D:44:ARG:HD2	1:F:51:GLU:HG3	1.84	0.58
1:D:10:VAL:HG21	1:F:133:TYR:CE2	2.38	0.58
1:D:48:LEU:N	1:D:48:LEU:HD22	2.19	0.58
1:D:97:TYR:HD2	1:D:114:PHE:CE1	2.20	0.58
1:F:56:ALA:HA	1:F:101:TYR:HD2	1.67	0.58
1:A:132:ASN:ND2	1:A:136:ILE:HD11	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:PHE:HD1	1:C:124:LEU:HD13	1.68	0.58
2:C:501:3CS:O35	2:C:501:3CS:H382	2.04	0.58
1:D:45:THR:OG1	1:F:44:ARG:HB2	2.03	0.58
1:C:139:PHE:CD1	1:C:139:PHE:N	2.71	0.58
1:E:120:LEU:HD23	2:E:506:3CS:C30	2.34	0.58
1:B:44:ARG:NH2	1:C:44:ARG:HH22	2.01	0.58
1:B:135:LEU:HD23	1:B:135:LEU:N	2.18	0.58
1:E:6:VAL:O	1:E:10:VAL:HG23	2.04	0.57
1:A:81:VAL:HB	1:A:82:PRO:CD	2.34	0.57
1:B:77:LEU:O	1:B:78:CYS:HB3	2.03	0.57
1:B:144:GLU:HA	1:B:144:GLU:OE1	2.02	0.57
1:D:116:LYS:HZ2	1:D:116:LYS:HB3	1.70	0.57
1:B:97:TYR:HD2	1:B:114:PHE:CD2	2.22	0.57
1:A:8:ASN:HA	1:A:80:GLN:OE1	2.03	0.57
1:B:144:GLU:HG3	1:B:146:TYR:CE1	2.40	0.57
1:B:145:ASN:O	1:B:147:ILE:HG13	2.04	0.57
1:C:90:TYR:HA	1:C:118:ILE:HD12	1.87	0.57
1:E:30:VAL:CG2	1:E:53:VAL:HG12	2.32	0.57
1:E:119:ILE:HD11	2:E:506:3CS:C12	2.35	0.57
1:E:123:PHE:HD1	1:E:124:LEU:HD13	1.70	0.57
1:A:33:GLU:HB3	1:A:50:PHE:HB2	1.86	0.57
1:A:125:MSE:O	1:A:128:ALA:HB3	2.04	0.57
1:D:30:VAL:HG11	1:F:112:TYR:CD2	2.39	0.57
1:C:56:ALA:HA	1:C:101:TYR:CD2	2.40	0.57
1:C:89:MSE:O	1:C:93:VAL:HG23	2.05	0.57
1:D:18:ILE:CG2	1:D:91:LEU:HD23	2.35	0.57
1:E:14:ILE:HG22	1:E:15:VAL:N	2.19	0.57
1:B:133:TYR:CD1	1:B:134:TYR:CD1	2.93	0.57
1:A:43:GLN:NE2	1:C:51:GLU:O	2.38	0.57
1:B:14:ILE:HG22	1:B:15:VAL:N	2.19	0.57
1:D:120:LEU:CD2	2:D:505:3CS:H301	2.31	0.57
1:D:136:ILE:O	1:D:140:GLY:HA3	2.04	0.57
1:E:97:TYR:HD2	1:E:114:PHE:CE2	2.22	0.57
1:B:47:THR:HA	1:B:51:GLU:CD	2.24	0.56
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.70	0.56
1:D:101:TYR:HD1	1:D:109:THR:CG2	2.16	0.56
1:C:63:ALA:C	1:C:65:PRO:HD2	2.25	0.56
1:D:42:PHE:N	1:D:42:PHE:HD1	2.03	0.56
1:A:42:PHE:CD1	1:C:112:TYR:CE1	2.93	0.56
2:D:505:3CS:H341	1:E:21:VAL:HG22	1.86	0.56
2:E:506:3CS:I25	1:F:25:PHE:HB2	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:ALA:HB2	1:F:101:TYR:CD2	2.40	0.56
2:F:504:3CS:C23	2:F:504:3CS:H371	2.35	0.56
1:D:14:ILE:HG22	1:D:15:VAL:N	2.19	0.56
1:E:53:VAL:HG23	1:E:102:LEU:HD23	1.87	0.56
1:A:21:VAL:HG12	1:A:22:GLN:N	2.20	0.56
1:D:11:LEU:HD23	1:D:80:GLN:HE22	1.70	0.56
1:A:42:PHE:HB2	1:C:112:TYR:OH	2.05	0.56
1:A:120:LEU:CD1	1:A:124:LEU:HD21	2.36	0.56
2:B:502:3CS:H20	1:C:24:GLY:C	2.26	0.56
1:D:35:ARG:HH21	1:D:39:GLY:HA2	1.71	0.56
1:A:13:ALA:O	1:A:17:LEU:HD23	2.05	0.56
1:B:44:ARG:O	1:B:44:ARG:HG3	2.05	0.56
1:D:123:PHE:CD2	2:D:505:3CS:H311	2.40	0.56
1:E:79:SER:OG	1:E:82:PRO:HD2	2.05	0.56
1:E:95:GLN:OE1	1:E:95:GLN:HA	2.04	0.56
1:E:135:LEU:HD23	1:E:135:LEU:N	2.20	0.56
1:C:14:ILE:HG22	1:C:15:VAL:N	2.21	0.56
1:D:30:VAL:HG11	1:F:112:TYR:CE2	2.41	0.56
1:E:30:VAL:HA	1:E:53:VAL:HG11	1.88	0.56
1:F:120:LEU:HA	2:F:504:3CS:H313	1.87	0.56
1:A:34:SER:HG	1:A:42:PHE:HE2	1.54	0.56
1:B:18:ILE:CG2	1:B:91:LEU:HD23	2.36	0.56
1:B:35:ARG:HE	1:B:35:ARG:HA	1.70	0.56
1:D:11:LEU:CD2	1:D:80:GLN:HE22	2.18	0.56
1:D:44:ARG:HD3	1:F:55:THR:OG1	2.05	0.56
1:E:72:TRP:O	1:E:76:LEU:HD22	2.05	0.56
1:F:31:GLU:O	1:F:35:ARG:HG2	2.06	0.56
1:B:142:ASP:O	1:B:143:PHE:HD1	1.89	0.55
1:C:120:LEU:HD13	1:C:124:LEU:HD21	1.87	0.55
1:D:11:LEU:HD23	1:D:80:GLN:CD	2.26	0.55
1:E:22:GLN:OE1	1:E:94:ARG:NE	2.39	0.55
1:E:54:TYR:HD2	1:F:42:PHE:HE2	1.54	0.55
1:A:63:ALA:CB	1:A:114:PHE:HE1	2.19	0.55
1:A:121:PHE:CE1	1:A:125:MSE:HG3	2.41	0.55
1:B:99:VAL:HG12	1:B:100:GLY:N	2.21	0.55
1:B:137:PHE:CE2	1:B:138:PHE:HE1	2.24	0.55
1:B:21:VAL:HG12	1:B:22:GLN:N	2.21	0.55
1:B:97:TYR:HD1	1:B:109:THR:HG21	1.70	0.55
1:C:11:LEU:HD23	1:C:80:GLN:HG3	1.88	0.55
1:E:60:CYS:HB3	1:E:94:ARG:HD3	1.88	0.55
1:F:37:GLN:OE1	1:F:37:GLN:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:TYR:O	1:E:113:ILE:HB	2.07	0.55
1:A:20:VAL:HG22	1:C:66:THR:CG2	2.32	0.55
1:A:120:LEU:HD13	1:A:124:LEU:HD22	1.89	0.55
1:B:74:ALA:CB	1:B:125:MSE:HE2	2.29	0.55
1:B:118:ILE:HG22	1:B:119:ILE:N	2.22	0.55
1:D:141:SER:C	1:D:143:PHE:H	2.09	0.55
1:E:47:THR:HG23	1:E:50:PHE:HB3	1.89	0.55
1:A:58:GLN:HG3	1:A:58:GLN:O	2.07	0.55
1:B:12:LEU:HG	1:B:80:GLN:HE21	1.72	0.55
1:B:105:ARG:HH11	1:B:105:ARG:HB3	1.72	0.55
1:B:113:ILE:HG12	1:B:114:PHE:N	2.20	0.55
1:B:133:TYR:CE1	1:B:134:TYR:CD1	2.95	0.55
1:E:81:VAL:HG22	1:E:82:PRO:HD3	1.88	0.55
1:E:111:GLY:O	1:E:112:TYR:O	2.25	0.55
2:A:503:3CS:C4	1:B:27:ALA:HB2	2.37	0.55
1:B:120:LEU:HB2	2:B:502:3CS:O35	2.07	0.55
1:B:130:ILE:HD11	1:C:14:ILE:HD12	1.89	0.55
1:E:33:GLU:HB3	1:E:50:PHE:HB2	1.88	0.55
1:E:64:TYR:CZ	1:E:68:LEU:HD21	2.41	0.55
1:A:31:GLU:OE1	1:A:31:GLU:HA	2.07	0.55
1:A:34:SER:O	1:A:37:GLN:O	2.24	0.55
1:B:10:VAL:HG13	1:B:14:ILE:HD12	1.88	0.55
1:C:18:ILE:HG22	1:C:91:LEU:HD23	1.88	0.55
1:D:11:LEU:HD23	1:D:80:GLN:OE1	2.07	0.55
1:D:30:VAL:CG2	1:D:53:VAL:HG12	2.37	0.55
1:E:120:LEU:HD23	2:E:506:3CS:H322	1.89	0.55
1:A:14:ILE:CD1	1:C:130:ILE:HD11	2.37	0.54
1:B:104:GLU:O	1:B:105:ARG:HB2	2.07	0.54
1:C:120:LEU:CD1	1:C:124:LEU:HD21	2.37	0.54
1:D:30:VAL:HA	1:D:53:VAL:HG11	1.88	0.54
2:D:505:3CS:O35	2:D:505:3CS:H382	2.07	0.54
1:A:43:GLN:HA	1:C:44:ARG:HH21	1.72	0.54
1:F:88:LEU:C	1:F:88:LEU:HD13	2.28	0.54
1:E:67:PHE:CD1	1:E:90:TYR:HD2	2.24	0.54
1:A:24:GLY:C	2:C:501:3CS:H20	2.28	0.54
1:E:66:THR:CG2	1:F:20:VAL:HG22	2.37	0.54
1:F:30:VAL:HG22	1:F:53:VAL:HG12	1.89	0.54
1:B:114:PHE:N	1:B:114:PHE:CD1	2.76	0.54
1:D:8:ASN:N	1:D:8:ASN:HD22	2.05	0.54
1:D:18:ILE:HG21	1:D:91:LEU:HD23	1.90	0.54
1:E:120:LEU:HD13	1:E:124:LEU:HD21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ASN:ND2	1:E:136:ILE:HD11	2.22	0.54
1:F:64:TYR:N	1:F:65:PRO:HD2	2.22	0.54
1:A:67:PHE:HB2	1:A:90:TYR:CE2	2.39	0.54
1:A:67:PHE:CG	1:A:90:TYR:CE2	2.96	0.54
1:E:130:ILE:HD11	1:F:14:ILE:CD1	2.38	0.54
1:F:94:ARG:HG2	1:F:114:PHE:CE2	2.42	0.54
1:A:18:ILE:CG2	1:A:91:LEU:HD23	2.37	0.54
2:B:502:3CS:H371	2:B:502:3CS:C19	2.38	0.54
1:C:21:VAL:HG12	1:C:22:GLN:N	2.22	0.54
1:C:119:ILE:CG1	2:C:501:3CS:H12	2.38	0.54
1:D:113:ILE:HG12	1:D:114:PHE:N	2.23	0.54
1:E:67:PHE:CD1	1:E:90:TYR:CD2	2.95	0.54
1:F:131:PHE:CD1	1:F:132:ASN:N	2.75	0.54
1:B:44:ARG:NE	1:C:44:ARG:HH12	2.05	0.54
1:C:106:THR:HG22	1:C:107:GLN:H	1.72	0.54
1:E:120:LEU:HD23	2:E:506:3CS:H301	1.89	0.54
2:E:506:3CS:H20	1:F:24:GLY:HA3	1.90	0.54
1:A:139:PHE:N	1:A:139:PHE:CD1	2.74	0.54
1:E:88:LEU:HD13	1:E:88:LEU:C	2.28	0.54
1:E:120:LEU:CD1	1:E:124:LEU:HD21	2.38	0.54
1:B:139:PHE:CD1	1:B:139:PHE:N	2.76	0.54
1:D:42:PHE:CD1	1:F:101:TYR:CZ	2.96	0.54
1:D:94:ARG:CD	1:D:114:PHE:HZ	2.21	0.54
2:D:505:3CS:H341	1:E:21:VAL:CG2	2.38	0.54
1:C:18:ILE:HG21	1:C:91:LEU:HD23	1.89	0.53
1:D:62:ASP:N	1:D:62:ASP:OD1	2.39	0.53
1:E:120:LEU:HD23	2:E:506:3CS:O35	2.08	0.53
1:F:19:SER:CB	1:F:91:LEU:HD11	2.33	0.53
1:F:79:SER:HB2	1:F:82:PRO:HD2	1.89	0.53
1:F:143:PHE:C	1:F:143:PHE:CD1	2.81	0.53
1:F:143:PHE:C	1:F:143:PHE:HD1	2.10	0.53
1:C:101:TYR:O	1:C:102:LEU:HD23	2.08	0.53
1:D:7:GLY:HA2	1:F:133:TYR:CE2	2.44	0.53
1:E:97:TYR:CE2	1:E:114:PHE:CE1	2.95	0.53
1:A:67:PHE:CD1	1:A:90:TYR:CD2	2.96	0.53
1:A:89:MSE:O	1:A:93:VAL:HG23	2.08	0.53
1:B:79:SER:HB3	1:B:82:PRO:CD	2.38	0.53
1:C:95:GLN:HA	1:C:95:GLN:OE1	2.07	0.53
1:D:44:ARG:HD2	1:F:51:GLU:CG	2.38	0.53
1:B:66:THR:CG2	1:C:20:VAL:HG22	2.38	0.53
1:B:96:LYS:HD2	1:B:96:LYS:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:PHE:N	1:D:143:PHE:CD1	2.75	0.53
1:F:76:LEU:HD13	1:F:76:LEU:N	2.23	0.53
1:D:45:THR:CG2	1:D:46:GLY:H	2.21	0.53
1:D:110:PRO:CG	1:E:40:ARG:HD3	2.38	0.53
1:F:143:PHE:O	1:F:144:GLU:O	2.27	0.53
1:A:43:GLN:OE1	1:C:44:ARG:O	2.26	0.53
2:C:501:3CS:C8	2:C:501:3CS:H13	2.39	0.53
1:F:121:PHE:CD1	1:F:121:PHE:C	2.80	0.53
1:A:15:VAL:HG13	1:A:16:THR:N	2.23	0.53
1:A:113:ILE:CD1	1:B:31:GLU:HG2	2.38	0.53
1:B:114:PHE:N	1:B:114:PHE:HD1	2.05	0.53
1:F:5:THR:O	1:F:9:VAL:HG13	2.08	0.53
1:D:22:GLN:HG3	1:D:23:ASN:N	2.24	0.53
1:D:42:PHE:HE1	1:F:110:PRO:HG2	1.73	0.53
1:F:33:GLU:OE1	1:F:33:GLU:HA	2.09	0.53
1:F:120:LEU:HD22	2:F:504:3CS:H313	1.91	0.53
1:A:14:ILE:HD12	1:C:130:ILE:HD11	1.90	0.53
1:D:120:LEU:CD1	1:D:124:LEU:HD21	2.39	0.53
1:E:97:TYR:CD2	1:E:114:PHE:CE2	2.97	0.53
1:F:34:SER:O	1:F:38:ASN:OD1	2.27	0.53
1:F:116:LYS:O	1:F:119:ILE:HD13	2.09	0.53
1:D:40:ARG:O	1:D:41:SER:HB2	2.09	0.53
2:E:506:3CS:C5	1:F:27:ALA:HB2	2.39	0.53
1:F:60:CYS:HG	1:F:114:PHE:HE1	1.57	0.53
1:B:81:VAL:CG1	1:B:82:PRO:HD3	2.34	0.52
1:B:102:LEU:HD13	1:B:104:GLU:OE2	2.09	0.52
1:D:44:ARG:HB3	1:E:44:ARG:HH22	1.72	0.52
1:E:133:TYR:CD1	1:E:134:TYR:CD1	2.97	0.52
1:A:3:GLN:NE2	1:C:133:TYR:CE1	2.77	0.52
1:A:88:LEU:C	1:A:88:LEU:HD13	2.29	0.52
1:C:22:GLN:HG3	1:C:23:ASN:N	2.24	0.52
1:C:25:PHE:CD1	1:C:25:PHE:C	2.82	0.52
1:A:63:ALA:C	1:A:65:PRO:HD2	2.29	0.52
1:D:139:PHE:CD1	1:D:139:PHE:N	2.76	0.52
1:B:119:ILE:HD13	1:B:119:ILE:H	1.75	0.52
1:B:137:PHE:CD2	1:B:138:PHE:CE1	2.98	0.52
1:C:13:ALA:O	1:C:17:LEU:HD23	2.09	0.52
1:E:58:GLN:O	1:E:58:GLN:HG3	2.10	0.52
1:F:25:PHE:CD1	1:F:25:PHE:C	2.82	0.52
1:A:96:LYS:HD2	1:A:96:LYS:H	1.71	0.52
1:B:31:GLU:HA	1:B:31:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ARG:HG2	1:D:114:PHE:CE1	2.45	0.52
1:A:25:PHE:CD1	1:A:25:PHE:C	2.81	0.52
1:A:64:TYR:N	1:A:65:PRO:HD2	2.25	0.52
1:B:30:VAL:HA	1:B:53:VAL:HG11	1.91	0.52
1:B:48:LEU:O	1:B:50:PHE:N	2.42	0.52
1:D:124:LEU:HD13	1:D:124:LEU:N	2.25	0.52
1:E:64:TYR:CE1	1:E:68:LEU:HD22	2.45	0.52
1:F:75:GLY:C	1:F:76:LEU:HD13	2.30	0.52
1:B:131:PHE:CD1	1:B:132:ASN:N	2.78	0.52
1:C:8:ASN:N	1:C:8:ASN:HD22	2.07	0.52
1:F:133:TYR:C	1:F:133:TYR:HD1	2.12	0.52
1:A:23:ASN:OD1	1:A:94:ARG:NH2	2.42	0.52
1:B:79:SER:HB3	1:B:82:PRO:HD2	1.91	0.52
1:C:71:LEU:O	1:C:71:LEU:HD22	2.10	0.52
1:C:136:ILE:HA	1:C:140:GLY:HA3	1.92	0.52
1:F:97:TYR:HD1	1:F:97:TYR:O	1.92	0.52
1:A:26:PHE:HB3	1:A:57:ASN:HD22	1.74	0.52
1:B:19:SER:O	1:B:23:ASN:HB2	2.10	0.52
1:D:42:PHE:O	1:D:43:GLN:HG3	2.10	0.52
1:F:135:LEU:N	1:F:135:LEU:HD23	2.25	0.52
1:A:42:PHE:N	1:A:42:PHE:HD1	2.08	0.52
1:F:58:GLN:O	1:F:58:GLN:HG3	2.08	0.52
1:D:52:ARG:HH11	1:D:52:ARG:CG	2.23	0.51
1:A:104:GLU:O	1:A:105:ARG:HB2	2.10	0.51
1:B:126:SER:O	1:B:130:ILE:HB	2.10	0.51
1:E:21:VAL:HG12	1:E:22:GLN:N	2.24	0.51
1:F:94:ARG:HG2	1:F:114:PHE:CZ	2.45	0.51
1:F:120:LEU:HD13	1:F:120:LEU:C	2.30	0.51
1:D:133:TYR:CD1	1:D:134:TYR:CD1	2.98	0.51
1:F:81:VAL:HG22	1:F:82:PRO:N	2.24	0.51
1:A:97:TYR:HD2	1:A:114:PHE:CG	2.27	0.51
1:C:63:ALA:CB	1:C:114:PHE:CE2	2.93	0.51
1:C:116:LYS:HA	1:C:119:ILE:CD1	2.41	0.51
1:D:71:LEU:HD22	1:D:71:LEU:O	2.10	0.51
1:D:110:PRO:HG3	1:E:40:ARG:O	2.10	0.51
2:D:505:3CS:H21	1:E:25:PHE:HB2	1.91	0.51
1:E:131:PHE:CD1	1:E:132:ASN:N	2.78	0.51
1:F:10:VAL:O	1:F:14:ILE:HD12	2.10	0.51
1:F:14:ILE:HG22	1:F:15:VAL:N	2.23	0.51
1:F:119:ILE:HG12	1:F:120:LEU:N	2.24	0.51
1:D:31:GLU:HA	1:D:31:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ALA:HB2	1:D:125:MSE:CE	2.35	0.51
1:F:13:ALA:O	1:F:17:LEU:HD23	2.11	0.51
1:F:79:SER:CB	1:F:82:PRO:HD2	2.40	0.51
1:A:10:VAL:O	1:A:14:ILE:HD12	2.11	0.51
1:C:139:PHE:N	1:C:139:PHE:HD1	2.09	0.51
1:E:11:LEU:CD2	1:E:80:GLN:HE22	2.24	0.51
1:E:67:PHE:CG	1:E:90:TYR:CE2	2.99	0.51
1:D:18:ILE:HG22	1:D:19:SER:N	2.26	0.51
1:D:90:TYR:CE1	1:D:94:ARG:HG3	2.46	0.51
1:D:90:TYR:HA	1:D:118:ILE:HD12	1.92	0.51
1:E:120:LEU:CD2	2:E:506:3CS:H322	2.41	0.51
1:A:17:LEU:O	1:A:20:VAL:HG12	2.11	0.51
1:B:14:ILE:O	1:B:18:ILE:HD12	2.10	0.51
1:B:125:MSE:O	1:B:128:ALA:HB3	2.11	0.51
1:C:116:LYS:O	1:C:119:ILE:HD13	2.10	0.51
1:D:3:GLN:NE2	1:F:133:TYR:CD1	2.79	0.51
1:D:131:PHE:CD1	1:D:132:ASN:N	2.79	0.51
2:F:504:3CS:H301	2:F:504:3CS:C37	2.27	0.51
1:C:114:PHE:CD1	1:C:115:GLY:N	2.78	0.50
1:D:25:PHE:HE2	1:D:95:GLN:HE22	1.59	0.50
1:D:97:TYR:HD2	1:D:114:PHE:CD1	2.29	0.50
1:D:116:LYS:HZ3	1:D:116:LYS:CA	2.22	0.50
1:E:8:ASN:N	1:E:8:ASN:HD22	2.07	0.50
1:E:47:THR:HG23	1:E:50:PHE:CB	2.41	0.50
1:F:26:PHE:CD2	1:F:98:PHE:CD2	2.99	0.50
1:A:42:PHE:HD1	1:A:42:PHE:H	1.60	0.50
2:A:503:3CS:C21	1:B:25:PHE:HB2	2.40	0.50
1:B:33:GLU:HA	1:B:33:GLU:OE1	2.11	0.50
1:E:64:TYR:N	1:E:65:PRO:HD2	2.25	0.50
1:A:14:ILE:HD11	1:C:130:ILE:CD1	2.41	0.50
1:A:22:GLN:HG3	1:A:23:ASN:N	2.26	0.50
1:D:64:TYR:CZ	1:D:68:LEU:HD21	2.46	0.50
1:B:133:TYR:CD1	1:B:134:TYR:HD1	2.29	0.50
1:E:79:SER:OG	1:E:80:GLN:N	2.44	0.50
1:A:43:GLN:NE2	1:C:54:TYR:HB3	2.23	0.50
1:A:135:LEU:N	1:A:135:LEU:HD23	2.27	0.50
1:B:72:TRP:O	1:B:76:LEU:HD22	2.12	0.50
1:D:58:GLN:O	1:D:58:GLN:HG3	2.11	0.50
1:D:79:SER:HB3	1:D:82:PRO:CD	2.42	0.50
1:D:116:LYS:HA	1:D:116:LYS:NZ	2.21	0.50
1:B:64:TYR:N	1:B:65:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ILE:HG22	1:C:19:SER:N	2.26	0.50
1:D:143:PHE:N	1:D:143:PHE:HD1	2.09	0.50
1:C:96:LYS:HD2	1:C:96:LYS:H	1.72	0.50
1:F:14:ILE:O	1:F:18:ILE:HD12	2.12	0.50
1:A:95:GLN:HA	1:A:95:GLN:OE1	2.11	0.50
1:B:64:TYR:CZ	1:B:68:LEU:CD2	2.95	0.50
1:B:97:TYR:CD1	1:B:109:THR:HG21	2.46	0.50
1:B:116:LYS:HE2	2:B:502:3CS:H383	1.93	0.50
1:B:133:TYR:HE1	1:B:134:TYR:CE1	2.30	0.50
1:C:74:ALA:CB	1:C:125:MSE:HE2	2.34	0.50
1:D:105:ARG:O	1:D:107:GLN:HG3	2.12	0.50
1:E:74:ALA:HB2	1:E:122:LEU:O	2.12	0.50
1:F:79:SER:HB2	1:F:82:PRO:CD	2.42	0.50
1:D:141:SER:O	1:D:142:ASP:OD1	2.29	0.49
1:E:10:VAL:HG13	1:E:14:ILE:HD12	1.92	0.49
1:E:45:THR:HB	1:F:43:GLN:NE2	2.27	0.49
1:E:119:ILE:CD1	2:E:506:3CS:H12	2.42	0.49
1:B:119:ILE:CG1	2:B:502:3CS:H12	2.42	0.49
1:D:21:VAL:HG12	1:D:22:GLN:N	2.26	0.49
1:F:64:TYR:CZ	1:F:68:LEU:HD21	2.47	0.49
1:B:112:TYR:HD2	1:C:30:VAL:CG1	2.24	0.49
1:B:120:LEU:HD13	1:B:120:LEU:C	2.31	0.49
1:D:74:ALA:HB2	1:D:122:LEU:O	2.12	0.49
1:D:109:THR:N	1:D:110:PRO:HD3	2.26	0.49
1:E:54:TYR:CD2	1:F:42:PHE:HE2	2.29	0.49
1:E:130:ILE:HD11	1:F:14:ILE:HD12	1.95	0.49
1:B:123:PHE:HD1	1:B:124:LEU:HD13	1.76	0.49
1:E:112:TYR:CD2	1:F:30:VAL:HG11	2.48	0.49
1:A:30:VAL:HA	1:A:53:VAL:HG11	1.95	0.49
1:E:105:ARG:O	1:E:106:THR:HB	2.12	0.49
1:D:7:GLY:HA2	1:F:133:TYR:OH	2.13	0.49
1:E:62:ASP:OD1	1:E:62:ASP:N	2.42	0.49
1:A:25:PHE:N	2:C:501:3CS:H21	2.28	0.49
2:A:503:3CS:H301	2:A:503:3CS:H372	1.94	0.49
1:B:130:ILE:HD12	1:C:14:ILE:HD11	1.94	0.49
1:D:101:TYR:CD1	1:D:109:THR:CG2	2.92	0.49
1:F:34:SER:HB2	1:F:50:PHE:HE1	1.77	0.49
1:F:124:LEU:O	1:F:127:VAL:HG12	2.11	0.49
1:A:26:PHE:CD1	1:A:26:PHE:N	2.81	0.49
1:C:33:GLU:HG3	1:C:50:PHE:CA	2.42	0.49
2:A:503:3CS:H371	2:A:503:3CS:C23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:LEU:CD1	1:C:77:LEU:N	2.75	0.49
1:E:52:ARG:HD3	1:E:104:GLU:OE1	2.13	0.49
1:F:97:TYR:CD2	1:F:114:PHE:CE1	3.01	0.49
1:A:57:ASN:C	1:A:59:ASN:H	2.15	0.48
2:A:503:3CS:H13	2:A:503:3CS:N26	2.28	0.48
1:B:120:LEU:HA	2:B:502:3CS:C31	2.39	0.48
1:E:78:CYS:HB3	1:E:125:MSE:HE3	1.95	0.48
1:A:124:LEU:O	1:A:127:VAL:HG12	2.13	0.48
1:D:41:SER:OG	1:F:110:PRO:HD2	2.13	0.48
1:D:116:LYS:NZ	1:D:116:LYS:CB	2.77	0.48
1:A:26:PHE:HD1	1:A:26:PHE:H	1.61	0.48
1:A:75:GLY:HA2	1:A:83:ALA:CB	2.43	0.48
1:C:11:LEU:O	1:C:15:VAL:HG12	2.13	0.48
1:C:77:LEU:O	1:C:129:GLY:HA3	2.12	0.48
1:D:116:LYS:NZ	2:D:505:3CS:C12	2.76	0.48
1:D:119:ILE:HG12	1:D:120:LEU:N	2.27	0.48
1:F:63:ALA:C	1:F:65:PRO:HD2	2.34	0.48
1:A:94:ARG:HG2	1:A:114:PHE:CZ	2.48	0.48
1:B:26:PHE:CD2	1:B:98:PHE:CD2	3.02	0.48
1:B:130:ILE:HD11	1:C:14:ILE:CD1	2.43	0.48
1:E:7:GLY:C	1:E:9:VAL:H	2.16	0.48
1:A:112:TYR:OH	1:B:27:ALA:HA	2.13	0.48
1:F:99:VAL:HG12	1:F:100:GLY:N	2.29	0.48
1:A:26:PHE:N	1:A:26:PHE:HD1	2.12	0.48
1:B:18:ILE:HG22	1:B:19:SER:N	2.28	0.48
1:B:47:THR:HA	1:B:51:GLU:CG	2.44	0.48
1:D:136:ILE:HA	1:D:140:GLY:CA	2.44	0.48
1:F:12:LEU:HB3	1:F:72:TRP:CH2	2.48	0.48
1:A:30:VAL:HG23	1:A:53:VAL:HG12	1.94	0.48
1:B:88:LEU:HD13	1:B:88:LEU:C	2.34	0.48
1:C:90:TYR:HD1	1:C:118:ILE:HG21	1.79	0.48
2:F:504:3CS:H371	2:F:504:3CS:C19	2.44	0.48
1:A:97:TYR:CD2	1:A:114:PHE:CG	3.02	0.48
1:B:44:ARG:CZ	1:C:44:ARG:HH12	2.27	0.48
1:B:133:TYR:CE1	1:B:134:TYR:HD1	2.31	0.48
1:E:96:LYS:HD2	1:E:96:LYS:H	1.74	0.48
1:C:114:PHE:CZ	2:C:501:3CS:C8	2.97	0.48
1:C:133:TYR:CE1	1:C:137:PHE:HB2	2.49	0.48
1:E:51:GLU:OE2	1:F:43:GLN:NE2	2.47	0.48
1:E:99:VAL:HG12	1:E:100:GLY:N	2.29	0.48
1:F:133:TYR:HA	1:F:136:ILE:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:HG21	1:B:91:LEU:HD23	1.96	0.48
1:B:60:CYS:HB3	1:B:94:ARG:HD3	1.94	0.48
1:D:26:PHE:CE2	1:D:98:PHE:HB2	2.49	0.48
1:E:90:TYR:N	1:E:118:ILE:CD1	2.77	0.48
1:F:42:PHE:HD1	1:F:43:GLN:H	1.60	0.48
1:A:26:PHE:CD2	1:A:98:PHE:CD2	3.02	0.47
1:A:85:PHE:O	1:A:88:LEU:HB3	2.14	0.47
1:B:97:TYR:CD2	1:B:114:PHE:CD2	3.00	0.47
1:D:10:VAL:O	1:D:14:ILE:HD12	2.14	0.47
1:A:11:LEU:HD23	1:A:80:GLN:CG	2.40	0.47
1:A:81:VAL:HB	1:A:82:PRO:HD3	1.96	0.47
2:A:503:3CS:N17	2:A:503:3CS:H393	2.28	0.47
1:B:141:SER:O	1:B:143:PHE:N	2.47	0.47
1:C:26:PHE:N	1:C:26:PHE:CD1	2.82	0.47
1:D:63:ALA:C	1:D:65:PRO:HD2	2.34	0.47
1:F:56:ALA:CB	1:F:101:TYR:CD2	2.97	0.47
2:A:503:3CS:C20	1:B:25:PHE:N	2.76	0.47
1:F:120:LEU:HD13	1:F:124:LEU:CD2	2.43	0.47
1:A:5:THR:O	1:A:9:VAL:HG13	2.13	0.47
1:B:130:ILE:CD1	1:C:14:ILE:HD11	2.44	0.47
1:C:25:PHE:O	1:C:25:PHE:HD1	1.97	0.47
1:D:124:LEU:O	1:D:127:VAL:HG12	2.14	0.47
1:F:121:PHE:HE1	1:F:125:MSE:HG3	1.79	0.47
1:A:19:SER:O	1:A:23:ASN:HB2	2.15	0.47
1:A:29:LYS:HD2	1:A:29:LYS:HA	1.62	0.47
1:A:118:ILE:HG22	1:A:119:ILE:N	2.30	0.47
1:B:25:PHE:HE1	1:B:29:LYS:HG2	1.77	0.47
1:B:71:LEU:HD22	1:B:71:LEU:C	2.34	0.47
1:B:132:ASN:O	1:B:136:ILE:HD12	2.14	0.47
1:C:29:LYS:HD2	1:C:29:LYS:HA	1.61	0.47
1:C:58:GLN:HG3	1:C:58:GLN:O	2.15	0.47
1:D:30:VAL:CG1	1:F:112:TYR:CD2	2.96	0.47
1:D:90:TYR:N	1:D:118:ILE:CD1	2.78	0.47
1:D:101:TYR:HD1	1:D:109:THR:HG22	1.75	0.47
1:D:119:ILE:HD11	2:D:505:3CS:C12	2.45	0.47
1:E:120:LEU:HA	2:E:506:3CS:H301	1.97	0.47
1:F:64:TYR:CZ	1:F:68:LEU:CD2	2.98	0.47
1:A:90:TYR:HD1	1:A:90:TYR:O	1.98	0.47
1:B:64:TYR:CE1	1:B:68:LEU:HD22	2.49	0.47
1:B:74:ALA:HB2	1:B:122:LEU:O	2.13	0.47
1:D:3:GLN:HE22	1:F:133:TYR:HD1	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:TYR:HE1	1:D:94:ARG:HG3	1.79	0.47
1:A:121:PHE:CD1	1:A:121:PHE:C	2.86	0.47
1:B:91:LEU:HD12	1:B:91:LEU:HA	1.72	0.47
1:C:26:PHE:HA	1:C:98:PHE:CE2	2.49	0.47
1:C:31:GLU:OE1	1:C:31:GLU:HA	2.15	0.47
1:C:115:GLY:O	1:C:119:ILE:HD12	2.14	0.47
1:D:37:GLN:O	1:D:38:ASN:HB2	2.14	0.47
1:D:123:PHE:HD1	1:D:124:LEU:CD1	2.27	0.47
1:E:63:ALA:C	1:E:65:PRO:HD2	2.35	0.47
1:F:12:LEU:O	1:F:15:VAL:HG12	2.14	0.47
1:F:31:GLU:OE1	1:F:31:GLU:HA	2.14	0.47
1:F:57:ASN:C	1:F:59:ASN:H	2.17	0.47
2:A:503:3CS:H20	1:B:24:GLY:C	2.35	0.47
1:B:39:GLY:O	1:B:42:PHE:N	2.48	0.47
1:B:102:LEU:C	1:B:102:LEU:HD22	2.35	0.47
1:D:116:LYS:HE3	2:D:505:3CS:C16	2.44	0.47
1:D:116:LYS:O	1:D:119:ILE:HD13	2.14	0.47
1:E:75:GLY:O	1:E:79:SER:O	2.33	0.47
1:F:62:ASP:OD1	1:F:62:ASP:N	2.47	0.47
1:A:64:TYR:CZ	1:A:68:LEU:CD2	2.98	0.47
1:B:142:ASP:OD2	1:F:117:ARG:NH1	2.35	0.47
1:E:45:THR:HA	1:F:43:GLN:NE2	2.29	0.47
2:E:506:3CS:H372	2:E:506:3CS:C32	2.33	0.47
1:C:76:LEU:HD12	1:C:76:LEU:HA	1.78	0.47
1:D:119:ILE:HD11	2:D:505:3CS:H12	1.96	0.47
1:E:11:LEU:CD2	1:E:80:GLN:NE2	2.78	0.47
1:E:11:LEU:HB2	1:E:80:GLN:NE2	2.29	0.47
1:A:94:ARG:CG	1:A:114:PHE:HE2	2.13	0.46
1:C:90:TYR:HD1	1:C:118:ILE:CG2	2.28	0.46
1:A:120:LEU:CD2	2:A:503:3CS:H313	2.45	0.46
1:A:133:TYR:CD1	1:A:134:TYR:CD1	3.02	0.46
1:A:133:TYR:CE1	1:A:134:TYR:CD1	3.03	0.46
1:C:18:ILE:HG22	1:C:91:LEU:CD2	2.45	0.46
1:D:48:LEU:HD22	1:D:48:LEU:H	1.81	0.46
1:D:106:THR:O	1:D:107:GLN:HB2	2.16	0.46
1:E:64:TYR:CZ	1:E:68:LEU:CD2	2.98	0.46
1:F:12:LEU:HD13	1:F:72:TRP:CE3	2.50	0.46
1:A:18:ILE:HG22	1:A:19:SER:N	2.30	0.46
1:B:105:ARG:O	1:B:106:THR:O	2.33	0.46
1:B:120:LEU:CD2	2:B:502:3CS:H313	2.46	0.46
1:C:124:LEU:O	1:C:127:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:LEU:HD23	2:F:504:3CS:H313	1.97	0.46
1:F:120:LEU:HB2	2:F:504:3CS:O35	2.14	0.46
1:A:124:LEU:O	1:A:128:ALA:N	2.49	0.46
1:B:21:VAL:CG1	1:B:22:GLN:N	2.79	0.46
1:B:52:ARG:HH11	1:B:52:ARG:CG	2.26	0.46
1:B:73:SER:O	1:B:77:LEU:HB2	2.15	0.46
1:D:29:LYS:HD2	1:D:29:LYS:HA	1.48	0.46
1:F:142:ASP:C	1:F:144:GLU:N	2.67	0.46
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.25	0.46
1:A:116:LYS:O	1:A:120:LEU:HB2	2.14	0.46
1:B:146:TYR:O	1:B:148:ALA:N	2.48	0.46
1:C:37:GLN:HG3	1:C:47:THR:OG1	2.15	0.46
1:D:31:GLU:CG	1:F:113:ILE:HD11	2.37	0.46
1:E:8:ASN:O	1:E:9:VAL:HG12	2.16	0.46
1:F:56:ALA:CA	1:F:101:TYR:CD2	2.97	0.46
2:F:504:3CS:H382	2:F:504:3CS:C29	2.45	0.46
1:A:9:VAL:N	1:A:80:GLN:NE2	2.63	0.46
1:A:90:TYR:N	1:A:118:ILE:CD1	2.78	0.46
1:B:22:GLN:HG3	1:B:23:ASN:N	2.29	0.46
1:E:95:GLN:O	1:E:99:VAL:HB	2.16	0.46
1:F:1:MSE:HB3	1:F:6:VAL:CG2	2.46	0.46
1:A:56:ALA:O	1:A:59:ASN:HB2	2.15	0.46
1:B:109:THR:N	1:B:110:PRO:CD	2.78	0.46
1:C:5:THR:O	1:C:9:VAL:HG13	2.15	0.46
1:E:77:LEU:CD1	1:E:77:LEU:N	2.78	0.46
1:A:27:ALA:HB2	2:C:501:3CS:C3	2.46	0.46
1:A:78:CYS:HB2	1:A:125:MSE:O	2.16	0.46
1:B:113:ILE:O	1:B:114:PHE:HB3	2.16	0.46
1:D:135:LEU:N	1:D:135:LEU:HD23	2.30	0.46
1:F:10:VAL:HG13	1:F:14:ILE:HD12	1.96	0.46
1:F:25:PHE:O	1:F:28:HIS:HB3	2.16	0.46
1:A:91:LEU:HD12	1:A:91:LEU:HA	1.78	0.46
1:C:35:ARG:HA	1:C:35:ARG:NE	2.28	0.46
1:E:18:ILE:CG2	1:E:91:LEU:HD23	2.46	0.46
1:E:67:PHE:CB	1:E:90:TYR:HE2	2.25	0.46
1:F:77:LEU:O	1:F:78:CYS:HB3	2.16	0.46
1:D:27:ALA:HB2	2:F:504:3CS:C3	2.46	0.46
1:D:116:LYS:CA	1:D:116:LYS:NZ	2.79	0.46
1:D:136:ILE:HA	1:D:140:GLY:HA3	1.98	0.46
1:E:91:LEU:HD12	1:E:91:LEU:HA	1.74	0.46
1:B:25:PHE:CE1	1:B:29:LYS:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:HA	1:B:35:ARG:NE	2.30	0.45
1:B:137:PHE:CD2	1:B:138:PHE:HE1	2.34	0.45
1:D:44:ARG:HB3	1:E:44:ARG:HH21	1.79	0.45
1:E:11:LEU:H	1:E:11:LEU:CD2	2.18	0.45
1:E:22:GLN:HG3	1:E:23:ASN:N	2.28	0.45
1:F:77:LEU:CD1	1:F:77:LEU:N	2.79	0.45
1:B:10:VAL:HG13	1:B:14:ILE:CD1	2.45	0.45
1:D:10:VAL:CG2	1:F:133:TYR:CD2	2.98	0.45
1:D:91:LEU:HD12	1:D:91:LEU:HA	1.75	0.45
1:E:26:PHE:CD2	1:E:98:PHE:CD2	3.04	0.45
1:E:90:TYR:HA	1:E:118:ILE:HD12	1.97	0.45
1:C:120:LEU:HD23	2:C:501:3CS:H323	1.99	0.45
1:D:133:TYR:CE1	1:D:134:TYR:CD1	3.05	0.45
1:E:18:ILE:HG22	1:E:19:SER:N	2.31	0.45
1:E:111:GLY:HA3	1:F:40:ARG:NH2	2.31	0.45
1:E:123:PHE:CE2	1:F:21:VAL:HG23	2.52	0.45
1:A:74:ALA:O	1:A:78:CYS:O	2.33	0.45
1:B:142:ASP:C	1:B:143:PHE:HD1	2.20	0.45
1:C:26:PHE:N	1:C:26:PHE:HD1	2.14	0.45
1:C:52:ARG:CG	1:C:52:ARG:HH11	2.30	0.45
1:E:83:ALA:CB	1:E:125:MSE:HE1	2.37	0.45
1:B:18:ILE:HG22	1:B:91:LEU:CD2	2.47	0.45
1:B:112:TYR:HD2	1:C:30:VAL:HG11	1.81	0.45
1:C:26:PHE:CD2	1:C:98:PHE:CD2	3.05	0.45
1:D:12:LEU:HG	1:D:80:GLN:HE21	1.81	0.45
1:D:90:TYR:HE1	1:D:94:ARG:CG	2.30	0.45
1:D:132:ASN:O	1:D:135:LEU:HB2	2.17	0.45
1:F:90:TYR:CD1	1:F:90:TYR:C	2.89	0.45
1:A:37:GLN:OE1	1:A:47:THR:HG21	2.16	0.45
1:A:42:PHE:CZ	1:C:112:TYR:HE1	2.34	0.45
1:A:132:ASN:HD21	1:A:136:ILE:HD11	1.81	0.45
1:D:12:LEU:O	1:D:15:VAL:HG12	2.17	0.45
1:D:67:PHE:HB2	1:D:90:TYR:CE2	2.52	0.45
1:D:79:SER:HB3	1:D:82:PRO:HD2	1.97	0.45
1:A:81:VAL:O	1:A:84:ALA:HB3	2.17	0.45
1:B:90:TYR:N	1:B:118:ILE:HD13	2.32	0.45
1:B:116:LYS:N	1:B:119:ILE:CD1	2.80	0.45
1:C:106:THR:CG2	1:C:107:GLN:H	2.30	0.45
1:C:106:THR:CG2	1:C:107:GLN:N	2.78	0.45
2:C:501:3CS:H182	2:C:501:3CS:C41	2.47	0.45
1:F:102:LEU:HD22	1:F:102:LEU:HA	1.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ALA:C	1:B:65:PRO:HD2	2.37	0.45
1:D:79:SER:C	1:D:82:PRO:HD2	2.37	0.45
1:D:81:VAL:N	1:D:82:PRO:CD	2.80	0.45
1:E:25:PHE:O	1:E:28:HIS:HB3	2.17	0.45
1:E:121:PHE:CE1	1:E:125:MSE:HG3	2.51	0.45
1:F:67:PHE:CD1	1:F:67:PHE:C	2.89	0.45
1:F:70:VAL:HG23	1:F:71:LEU:N	2.31	0.45
1:F:106:THR:O	1:F:107:GLN:HB2	2.16	0.45
1:A:3:GLN:NE2	1:C:133:TYR:CD1	2.85	0.45
1:A:18:ILE:HG21	1:A:91:LEU:HD23	1.98	0.45
1:A:42:PHE:CG	1:C:112:TYR:CE1	3.05	0.45
1:A:90:TYR:HE1	1:A:114:PHE:CE2	2.35	0.45
1:A:95:GLN:O	1:A:99:VAL:HB	2.17	0.45
1:A:124:LEU:HD13	1:A:124:LEU:N	2.31	0.45
1:B:106:THR:O	1:B:108:SER:N	2.50	0.45
1:A:56:ALA:HA	1:A:101:TYR:HD2	1.81	0.45
2:A:503:3CS:H382	2:A:503:3CS:C23	2.44	0.45
2:A:503:3CS:H13	2:A:503:3CS:C9	2.47	0.45
2:A:503:3CS:I25	1:B:25:PHE:HB2	2.87	0.45
1:B:139:PHE:CD2	1:F:121:PHE:HB2	2.52	0.45
1:D:64:TYR:N	1:D:65:PRO:HD2	2.32	0.45
1:E:22:GLN:CG	1:E:23:ASN:N	2.80	0.45
1:E:109:THR:N	1:E:110:PRO:HD3	2.32	0.45
1:E:130:ILE:CD1	1:F:14:ILE:HD11	2.47	0.45
2:E:506:3CS:H23	2:E:506:3CS:O42	2.16	0.45
1:A:76:LEU:HD12	1:A:76:LEU:HA	1.81	0.44
1:B:2:ASP:OD1	1:B:5:THR:HG23	2.17	0.44
1:C:11:LEU:CD2	1:C:80:GLN:NE2	2.69	0.44
1:C:116:LYS:HA	1:C:119:ILE:HD11	1.99	0.44
1:D:123:PHE:HB2	2:D:505:3CS:H313	1.98	0.44
1:E:56:ALA:HA	1:E:101:TYR:CD2	2.52	0.44
1:E:59:ASN:ND2	1:E:112:TYR:H	2.15	0.44
1:D:18:ILE:HG22	1:D:91:LEU:CD2	2.47	0.44
1:D:42:PHE:CE2	1:F:112:TYR:CA	3.01	0.44
1:D:79:SER:O	1:D:82:PRO:HD2	2.18	0.44
1:F:11:LEU:HD22	1:F:80:GLN:HE22	1.82	0.44
1:A:22:GLN:OE1	1:A:94:ARG:NE	2.49	0.44
1:A:137:PHE:CE2	1:A:138:PHE:HE1	2.36	0.44
1:B:77:LEU:N	1:B:77:LEU:CD1	2.80	0.44
1:D:2:ASP:OD2	1:D:5:THR:HG23	2.17	0.44
1:D:94:ARG:CG	1:D:114:PHE:CZ	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ARG:HD3	1:D:114:PHE:HZ	1.82	0.44
1:D:99:VAL:HG12	1:D:100:GLY:N	2.32	0.44
1:E:44:ARG:HH11	1:E:44:ARG:HB2	1.82	0.44
1:B:74:ALA:CB	1:B:122:LEU:HD12	2.48	0.44
1:C:133:TYR:CD1	1:C:133:TYR:C	2.90	0.44
1:A:102:LEU:CG	1:A:103:GLY:H	2.15	0.44
2:B:502:3CS:H21	1:C:25:PHE:N	2.32	0.44
1:C:64:TYR:N	1:C:65:PRO:HD2	2.33	0.44
1:D:6:VAL:HG12	1:F:133:TYR:CD2	2.52	0.44
1:D:15:VAL:O	1:D:18:ILE:HB	2.18	0.44
1:D:143:PHE:CE2	1:D:144:GLU:HG2	2.53	0.44
1:E:12:LEU:HD13	1:E:72:TRP:CE3	2.52	0.44
1:F:55:THR:HG21	1:F:101:TYR:OH	2.18	0.44
1:F:78:CYS:O	1:F:79:SER:CB	2.65	0.44
1:C:26:PHE:HD1	1:C:26:PHE:H	1.65	0.44
1:D:89:MSE:O	1:D:93:VAL:HG23	2.16	0.44
1:A:14:ILE:HD11	1:C:130:ILE:HD12	1.99	0.44
1:B:90:TYR:N	1:B:118:ILE:CD1	2.81	0.44
1:C:90:TYR:CD1	1:C:118:ILE:HG21	2.53	0.44
1:C:120:LEU:CD2	2:C:501:3CS:H323	2.47	0.44
1:D:66:THR:CG2	1:E:20:VAL:HG22	2.44	0.44
1:A:63:ALA:HB2	1:A:114:PHE:HE1	1.82	0.44
1:A:97:TYR:CD2	1:A:114:PHE:CB	3.01	0.44
1:B:90:TYR:CD1	1:B:90:TYR:C	2.91	0.44
1:D:47:THR:HG22	1:D:49:ALA:H	1.83	0.44
1:E:119:ILE:CG1	2:E:506:3CS:H12	2.48	0.44
1:F:52:ARG:HG3	1:F:52:ARG:NH1	2.29	0.44
1:F:121:PHE:HE1	1:F:125:MSE:CG	2.30	0.44
1:F:140:GLY:C	1:F:142:ASP:N	2.71	0.44
1:A:35:ARG:NH2	1:C:113:ILE:CD1	2.81	0.44
1:A:90:TYR:HB2	1:A:118:ILE:HG21	1.99	0.44
1:A:110:PRO:CB	1:B:42:PHE:HB2	2.48	0.44
1:B:110:PRO:HB3	1:C:35:ARG:HH22	1.83	0.44
1:B:144:GLU:CB	1:B:146:TYR:CE1	2.99	0.44
1:E:126:SER:HB2	1:F:17:LEU:HD11	2.00	0.44
1:A:90:TYR:HA	1:A:118:ILE:HD12	2.00	0.43
1:D:10:VAL:HG12	1:D:11:LEU:N	2.32	0.43
1:D:44:ARG:HE	1:D:44:ARG:CA	2.31	0.43
1:A:25:PHE:HD1	1:A:25:PHE:O	2.01	0.43
1:B:145:ASN:HD22	1:B:145:ASN:N	2.01	0.43
1:C:119:ILE:HD13	1:C:119:ILE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:ARG:HH11	1:F:51:GLU:HG2	1.81	0.43
1:E:80:GLN:H	1:E:82:PRO:HD2	1.83	0.43
1:E:133:TYR:CD1	1:E:134:TYR:HD1	2.34	0.43
1:F:97:TYR:HB3	1:F:114:PHE:CZ	2.53	0.43
1:A:67:PHE:CD1	1:A:90:TYR:HD2	2.36	0.43
1:B:130:ILE:CD1	1:C:14:ILE:CD1	2.96	0.43
1:C:87:GLY:O	1:C:90:TYR:HB3	2.19	0.43
1:D:52:ARG:CG	1:D:52:ARG:NH1	2.81	0.43
1:D:85:PHE:O	1:D:88:LEU:HB3	2.18	0.43
1:D:116:LYS:HZ3	1:D:119:ILE:HD11	1.83	0.43
1:E:90:TYR:HB2	1:E:118:ILE:HD13	2.00	0.43
1:E:133:TYR:CE1	1:E:134:TYR:CD1	3.07	0.43
1:F:64:TYR:CE1	1:F:68:LEU:HD22	2.53	0.43
1:A:111:GLY:HA2	1:B:31:GLU:CD	2.38	0.43
2:B:502:3CS:C21	1:C:25:PHE:N	2.81	0.43
1:C:7:GLY:C	1:C:9:VAL:H	2.22	0.43
1:C:33:GLU:CG	1:C:50:PHE:HA	2.48	0.43
1:D:57:ASN:C	1:D:59:ASN:H	2.21	0.43
1:F:104:GLU:OE1	1:F:104:GLU:HA	2.17	0.43
1:A:74:ALA:CB	1:A:122:LEU:HD12	2.49	0.43
1:C:22:GLN:HE21	1:C:22:GLN:HB2	1.67	0.43
1:C:81:VAL:N	1:C:82:PRO:CD	2.81	0.43
1:C:144:GLU:OE1	1:C:147:ILE:HD11	2.19	0.43
1:D:21:VAL:HG23	1:F:123:PHE:CE2	2.53	0.43
1:D:133:TYR:HD1	1:D:134:TYR:CD1	2.37	0.43
1:E:10:VAL:O	1:E:14:ILE:HD12	2.19	0.43
1:E:29:LYS:HD2	1:E:29:LYS:HA	1.55	0.43
1:A:30:VAL:HG23	1:A:53:VAL:CG1	2.48	0.43
1:F:1:MSE:HB3	1:F:6:VAL:HG22	1.99	0.43
1:F:29:LYS:HD2	1:F:29:LYS:HA	1.51	0.43
1:F:79:SER:HB2	1:F:82:PRO:HG2	2.01	0.43
1:D:10:VAL:CG2	1:F:133:TYR:CE2	3.00	0.43
1:E:74:ALA:HB1	1:E:125:MSE:HE2	2.00	0.43
1:F:22:GLN:HG3	1:F:23:ASN:N	2.33	0.43
1:B:26:PHE:CG	1:B:98:PHE:CD2	3.06	0.43
1:B:90:TYR:HA	1:B:118:ILE:HD13	1.99	0.43
1:B:124:LEU:HD13	1:B:124:LEU:N	2.34	0.43
1:D:26:PHE:N	1:D:26:PHE:CD1	2.87	0.43
2:E:506:3CS:C19	2:E:506:3CS:H371	2.49	0.43
1:F:12:LEU:HD11	1:F:75:GLY:HA3	1.99	0.43
1:F:90:TYR:N	1:F:118:ILE:CD1	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:HB2	1:C:51:GLU:OE1	2.19	0.43
1:B:56:ALA:HA	1:B:101:TYR:CD2	2.54	0.43
1:B:67:PHE:HB2	1:B:90:TYR:CE2	2.53	0.43
1:C:90:TYR:CB	1:C:118:ILE:HG21	2.46	0.43
1:E:47:THR:CG2	1:E:50:PHE:HB3	2.48	0.43
1:F:26:PHE:HB3	1:F:57:ASN:HD22	1.84	0.43
1:F:90:TYR:HD1	1:F:90:TYR:O	2.01	0.43
1:A:9:VAL:O	1:A:9:VAL:HG23	2.18	0.43
1:A:67:PHE:CD1	1:A:67:PHE:C	2.92	0.43
1:B:120:LEU:CD1	1:B:124:LEU:HD21	2.48	0.43
2:B:502:3CS:I25	1:C:25:PHE:HB2	2.88	0.43
1:D:120:LEU:HD23	2:D:505:3CS:C29	2.48	0.43
1:D:133:TYR:CD1	1:D:134:TYR:HD1	2.36	0.43
1:E:23:ASN:OD1	1:E:94:ARG:NH2	2.51	0.43
1:F:132:ASN:HD21	1:F:136:ILE:HD11	1.83	0.43
1:A:81:VAL:N	1:A:82:PRO:HD2	2.33	0.42
1:C:63:ALA:CB	1:C:114:PHE:CZ	3.02	0.42
1:C:63:ALA:HB1	1:C:114:PHE:CZ	2.53	0.42
1:C:131:PHE:CD1	1:C:132:ASN:N	2.87	0.42
1:D:2:ASP:OD1	1:D:2:ASP:N	2.51	0.42
1:D:124:LEU:HA	1:D:124:LEU:HD12	1.82	0.42
1:E:60:CYS:HG	1:E:114:PHE:HE2	1.63	0.42
1:A:90:TYR:C	1:A:90:TYR:CD1	2.93	0.42
1:B:30:VAL:CG2	1:B:53:VAL:CG1	2.97	0.42
1:B:144:GLU:O	1:F:89:MSE:HE3	2.19	0.42
1:C:1:MSE:HE3	1:C:5:THR:OG1	2.19	0.42
1:C:55:THR:HG22	1:C:101:TYR:CE2	2.54	0.42
1:D:42:PHE:CE2	1:F:111:GLY:C	2.93	0.42
1:E:133:TYR:HD1	1:E:134:TYR:CD1	2.36	0.42
1:C:83:ALA:HB2	1:C:125:MSE:CE	2.25	0.42
2:D:505:3CS:C21	1:E:25:PHE:HB2	2.49	0.42
1:F:132:ASN:ND2	1:F:136:ILE:HD11	2.34	0.42
1:B:48:LEU:O	1:B:51:GLU:N	2.52	0.42
1:B:102:LEU:HD23	1:B:102:LEU:HA	1.87	0.42
1:B:116:LYS:CA	1:B:119:ILE:HD11	2.50	0.42
1:A:11:LEU:HD13	1:A:11:LEU:N	2.34	0.42
2:A:503:3CS:C38	2:A:503:3CS:C23	2.96	0.42
1:B:18:ILE:HG22	1:B:91:LEU:HD23	2.00	0.42
1:B:135:LEU:C	1:B:137:PHE:H	2.22	0.42
1:C:135:LEU:HD23	1:C:135:LEU:HA	1.78	0.42
1:E:7:GLY:O	1:E:9:VAL:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:GLU:OE1	1:E:33:GLU:HA	2.20	0.42
1:B:133:TYR:CE1	1:B:134:TYR:CE1	3.08	0.42
1:B:144:GLU:CG	1:B:146:TYR:CE1	3.02	0.42
2:B:502:3CS:O42	2:B:502:3CS:H23	2.19	0.42
1:C:22:GLN:CG	1:C:23:ASN:N	2.82	0.42
1:D:47:THR:HB	1:D:50:PHE:HB3	2.02	0.42
1:E:52:ARG:HH11	1:E:52:ARG:CG	2.29	0.42
1:E:77:LEU:HD21	1:F:13:ALA:HB1	2.01	0.42
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.80	0.42
2:A:503:3CS:H182	2:A:503:3CS:H393	2.02	0.42
1:B:57:ASN:C	1:B:59:ASN:H	2.21	0.42
1:B:118:ILE:CG2	1:B:119:ILE:N	2.82	0.42
1:F:74:ALA:HB2	1:F:122:LEU:O	2.18	0.42
1:F:124:LEU:HA	1:F:124:LEU:HD12	1.78	0.42
2:A:503:3CS:H181	1:B:28:HIS:HB2	2.02	0.42
2:B:502:3CS:C21	1:C:25:PHE:CA	2.98	0.42
1:C:53:VAL:HG12	1:C:54:TYR:N	2.35	0.42
1:E:81:VAL:CB	1:E:82:PRO:HD3	2.50	0.42
1:A:126:SER:O	1:A:130:ILE:HB	2.19	0.42
1:B:90:TYR:C	1:B:90:TYR:HD1	2.24	0.42
1:B:133:TYR:HD1	1:B:134:TYR:CD1	2.38	0.42
1:B:138:PHE:N	1:B:138:PHE:CD1	2.87	0.42
1:D:90:TYR:CD1	1:D:90:TYR:C	2.94	0.42
1:E:85:PHE:CZ	1:E:89:MSE:CE	3.03	0.42
1:E:133:TYR:CE1	1:F:10:VAL:HG21	2.55	0.42
1:F:7:GLY:C	1:F:9:VAL:H	2.23	0.42
1:F:35:ARG:HA	1:F:38:ASN:OD1	2.19	0.42
1:F:124:LEU:C	1:F:127:VAL:HG12	2.40	0.42
1:A:11:LEU:CD2	1:A:80:GLN:NE2	2.80	0.42
1:A:15:VAL:CG1	1:A:16:THR:N	2.83	0.42
1:A:124:LEU:HA	1:A:124:LEU:HD12	1.87	0.42
1:B:29:LYS:HA	1:B:29:LYS:HD2	1.57	0.42
1:C:72:TRP:O	1:C:76:LEU:HD22	2.20	0.42
1:C:74:ALA:HB2	1:C:122:LEU:O	2.20	0.42
1:E:114:PHE:O	1:E:115:GLY:C	2.58	0.42
1:F:139:PHE:C	1:F:141:SER:H	2.20	0.42
1:C:124:LEU:C	1:C:127:VAL:HG12	2.40	0.41
1:D:22:GLN:CG	1:D:23:ASN:N	2.81	0.41
1:D:26:PHE:HD1	1:D:26:PHE:H	1.67	0.41
1:D:56:ALA:HB2	1:D:101:TYR:HB3	2.02	0.41
1:D:123:PHE:HD1	1:D:124:LEU:HD13	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PHE:CA	2:C:501:3CS:C21	2.98	0.41
1:B:116:LYS:HA	1:B:119:ILE:HD11	2.01	0.41
1:C:62:ASP:OD1	1:C:62:ASP:N	2.53	0.41
1:C:113:ILE:O	1:C:114:PHE:CG	2.73	0.41
1:A:42:PHE:CD2	1:A:50:PHE:CZ	2.96	0.41
1:B:50:PHE:HD1	1:B:50:PHE:O	2.03	0.41
1:B:85:PHE:HZ	1:B:89:MSE:HE2	1.85	0.41
1:C:85:PHE:O	1:C:88:LEU:HB3	2.20	0.41
1:C:135:LEU:O	1:C:139:PHE:N	2.53	0.41
1:D:67:PHE:CD1	1:D:67:PHE:C	2.91	0.41
1:D:88:LEU:C	1:D:88:LEU:HD13	2.40	0.41
1:D:108:SER:C	1:E:40:ARG:HD2	2.38	0.41
1:D:112:TYR:CE2	1:E:30:VAL:CG1	2.99	0.41
1:D:120:LEU:O	1:D:124:LEU:HD22	2.20	0.41
1:E:15:VAL:O	1:E:18:ILE:HB	2.20	0.41
1:E:48:LEU:HD13	1:E:48:LEU:C	2.40	0.41
1:B:107:GLN:CG	1:C:40:ARG:HD2	2.50	0.41
1:C:113:ILE:HG22	1:C:114:PHE:O	2.20	0.41
1:D:33:GLU:HA	1:D:33:GLU:OE1	2.21	0.41
1:F:64:TYR:O	1:F:67:PHE:HB3	2.20	0.41
1:A:12:LEU:O	1:A:15:VAL:HG12	2.21	0.41
1:D:116:LYS:NZ	2:D:505:3CS:C16	2.78	0.41
1:F:26:PHE:CE2	1:F:98:PHE:CD2	3.08	0.41
1:B:11:LEU:HD13	1:B:11:LEU:N	2.35	0.41
1:D:25:PHE:O	1:D:28:HIS:HB3	2.21	0.41
1:D:124:LEU:N	1:D:124:LEU:CD1	2.83	0.41
1:E:2:ASP:OD1	1:E:5:THR:HG23	2.21	0.41
1:E:44:ARG:H	1:E:44:ARG:HG2	1.44	0.41
1:E:68:LEU:HD12	1:E:68:LEU:HA	1.80	0.41
1:F:2:ASP:N	1:F:2:ASP:OD1	2.54	0.41
1:F:79:SER:OG	1:F:82:PRO:HD2	2.20	0.41
1:A:64:TYR:CE1	1:A:68:LEU:HD22	2.55	0.41
1:A:71:LEU:O	1:A:71:LEU:HD22	2.20	0.41
1:B:26:PHE:CD1	1:B:26:PHE:N	2.89	0.41
1:B:120:LEU:CD1	1:B:124:LEU:CD2	2.97	0.41
1:B:135:LEU:C	1:B:137:PHE:N	2.72	0.41
1:C:26:PHE:CE2	1:C:98:PHE:CD2	3.09	0.41
1:D:138:PHE:CD1	1:D:138:PHE:N	2.88	0.41
2:D:505:3CS:C21	1:E:25:PHE:CA	2.99	0.41
1:E:113:ILE:C	1:E:114:PHE:HD1	2.23	0.41
1:A:22:GLN:CG	1:A:23:ASN:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PRO:HG2	1:B:66:THR:H	1.84	0.41
1:D:124:LEU:C	1:D:127:VAL:HG12	2.41	0.41
1:E:55:THR:OG1	1:F:42:PHE:HD2	2.02	0.41
1:F:10:VAL:CG1	1:F:14:ILE:CD1	2.98	0.41
1:F:91:LEU:HD12	1:F:91:LEU:HA	1.78	0.41
1:F:121:PHE:HD1	1:F:121:PHE:O	2.04	0.41
1:A:8:ASN:C	1:A:9:VAL:HG12	2.41	0.41
1:A:25:PHE:N	2:C:501:3CS:C21	2.83	0.41
1:A:33:GLU:OE2	1:A:49:ALA:HB1	2.20	0.41
1:A:56:ALA:HA	1:A:101:TYR:CD2	2.56	0.41
1:A:133:TYR:CD1	1:A:133:TYR:C	2.94	0.41
1:B:26:PHE:CG	1:B:98:PHE:CE2	3.09	0.41
1:B:35:ARG:C	1:B:37:GLN:H	2.24	0.41
1:B:38:ASN:C	1:B:40:ARG:N	2.74	0.41
1:B:81:VAL:N	1:B:82:PRO:CD	2.84	0.41
1:B:112:TYR:CD2	1:C:30:VAL:CG1	2.97	0.41
1:C:10:VAL:HG13	1:C:14:ILE:HD13	2.00	0.41
1:C:95:GLN:O	1:C:99:VAL:HB	2.20	0.41
1:D:19:SER:HB2	1:D:64:TYR:CE1	2.56	0.41
1:D:78:CYS:HB2	1:D:125:MSE:O	2.21	0.41
1:E:22:GLN:HE21	1:E:22:GLN:HB2	1.72	0.41
1:E:52:ARG:CG	1:E:52:ARG:NH1	2.83	0.41
1:F:30:VAL:CG2	1:F:53:VAL:HG12	2.51	0.41
1:F:79:SER:O	1:F:80:GLN:CB	2.69	0.41
1:A:10:VAL:HG13	1:A:14:ILE:HD13	2.01	0.41
1:A:64:TYR:CE1	1:A:68:LEU:CD2	3.03	0.41
1:B:10:VAL:HG12	1:B:11:LEU:N	2.34	0.41
1:B:56:ALA:HB2	1:B:101:TYR:HB3	2.03	0.41
1:D:5:THR:O	1:D:9:VAL:HG13	2.21	0.41
1:D:25:PHE:CA	2:F:504:3CS:C21	2.99	0.41
1:D:74:ALA:CB	1:D:122:LEU:HD12	2.51	0.41
1:E:90:TYR:C	1:E:90:TYR:CD1	2.91	0.41
1:E:135:LEU:N	1:E:135:LEU:CD2	2.84	0.41
1:F:67:PHE:CG	1:F:90:TYR:HE2	2.37	0.41
1:F:146:TYR:O	1:F:147:ILE:HD13	2.21	0.41
1:A:97:TYR:CD2	1:A:114:PHE:HB3	2.56	0.40
1:B:25:PHE:CD1	1:B:25:PHE:C	2.94	0.40
1:D:116:LYS:CE	2:D:505:3CS:C16	3.00	0.40
1:D:121:PHE:CD1	1:D:121:PHE:C	2.94	0.40
1:E:64:TYR:CE1	1:E:68:LEU:CD2	3.03	0.40
1:F:33:GLU:OE2	1:F:49:ALA:HB1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:CYS:O	1:F:78:CYS:SG	2.79	0.40
1:A:10:VAL:HG21	1:C:133:TYR:HD2	1.80	0.40
1:C:147:ILE:HG22	1:C:147:ILE:O	2.20	0.40
2:E:506:3CS:C21	1:F:25:PHE:N	2.84	0.40
1:A:33:GLU:OE1	1:A:33:GLU:HA	2.21	0.40
1:A:40:ARG:HD3	1:C:52:ARG:HH22	1.86	0.40
1:A:42:PHE:CG	1:C:112:TYR:HE1	2.40	0.40
1:A:137:PHE:O	1:A:137:PHE:CD1	2.74	0.40
1:B:11:LEU:HD22	1:B:11:LEU:N	2.09	0.40
1:C:52:ARG:NE	1:C:102:LEU:HA	2.36	0.40
1:D:25:PHE:CE1	1:D:29:LYS:HG2	2.57	0.40
1:D:64:TYR:CZ	1:D:68:LEU:CD2	3.04	0.40
1:D:113:ILE:HG12	1:D:114:PHE:O	2.20	0.40
1:D:132:ASN:ND2	1:D:136:ILE:HD11	2.37	0.40
1:F:81:VAL:N	1:F:82:PRO:CD	2.84	0.40
1:A:22:GLN:NE2	1:A:26:PHE:CZ	2.89	0.40
1:D:11:LEU:HB2	1:D:80:GLN:NE2	2.36	0.40
1:D:133:TYR:CE1	1:D:134:TYR:HD1	2.40	0.40
1:E:8:ASN:C	1:E:9:VAL:CG1	2.89	0.40
1:E:45:THR:CB	1:F:43:GLN:NE2	2.85	0.40
1:A:11:LEU:HB3	1:A:84:ALA:CB	2.51	0.40
1:A:136:ILE:H	1:A:136:ILE:HG13	1.63	0.40
1:B:26:PHE:N	1:B:26:PHE:HD1	2.19	0.40
1:B:85:PHE:CD1	1:B:85:PHE:C	2.94	0.40
1:C:50:PHE:CD1	1:C:50:PHE:C	2.94	0.40
1:D:26:PHE:N	1:D:26:PHE:HD1	2.20	0.40
1:E:130:ILE:CD1	1:F:14:ILE:CD1	2.99	0.40
1:F:90:TYR:CE1	1:F:94:ARG:HG3	2.56	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	138/161 (86%)	108 (78%)	21 (15%)	9 (6%)	1 18
1	B	146/161 (91%)	98 (67%)	26 (18%)	22 (15%)	0 3
1	C	147/161 (91%)	115 (78%)	25 (17%)	7 (5%)	2 23
1	D	146/161 (91%)	109 (75%)	31 (21%)	6 (4%)	3 25
1	E	138/161 (86%)	110 (80%)	17 (12%)	11 (8%)	1 14
1	F	147/161 (91%)	107 (73%)	26 (18%)	14 (10%)	0 10
All	All	862/966 (89%)	647 (75%)	146 (17%)	69 (8%)	1 14

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	THR
1	B	39	GLY
1	B	42	PHE
1	B	45	THR
1	B	49	ALA
1	B	106	THR
1	B	143	PHE
1	C	41	SER
1	C	79	SER
1	C	109	THR
1	D	106	THR
1	E	104	GLU
1	E	112	TYR
1	E	115	GLY
1	F	40	ARG
1	F	79	SER
1	F	108	SER
1	F	144	GLU
1	A	103	GLY
1	B	37	GLN
1	B	41	SER
1	B	107	GLN
1	B	114	PHE
1	B	146	TYR
1	E	8	ASN
1	E	106	THR
1	E	110	PRO
1	E	111	GLY
1	E	113	ILE
1	F	80	GLN

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Mol	Chain	Res	Type
1	F	115	GLY
1	F	148	ALA
1	A	45	THR
1	A	80	GLN
1	B	8	ASN
1	B	79	SER
1	B	147	ILE
1	C	3	GLN
1	C	8	ASN
1	D	3	GLN
1	D	41	SER
1	D	104	GLU
1	D	143	PHE
1	E	80	GLN
1	F	134	TYR
1	A	8	ASN
1	A	128	ALA
1	B	47	THR
1	B	78	CYS
1	B	105	ARG
1	B	142	ASP
1	F	8	ASN
1	F	39	GLY
1	F	78	CYS
1	A	3	GLN
1	B	3	GLN
1	C	64	TYR
1	E	3	GLN
1	E	9	VAL
1	F	58	GLN
1	A	9	VAL
1	A	111	GLY
1	C	9	VAL
1	F	9	VAL
1	B	9	VAL
1	D	9	VAL
1	B	110	PRO
1	F	65	PRO
1	A	81	VAL

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	117/134 (87%)	67 (57%)	50 (43%)	0	0
1	B	124/134 (92%)	69 (56%)	55 (44%)	0	0
1	C	125/134 (93%)	83 (66%)	42 (34%)	0	2
1	D	124/134 (92%)	75 (60%)	49 (40%)	0	0
1	E	117/134 (87%)	67 (57%)	50 (43%)	0	0
1	F	125/134 (93%)	74 (59%)	51 (41%)	0	0
All	All	732/804 (91%)	435 (59%)	297 (41%)	0	0

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	8	ASN
1	A	10	VAL
1	A	11	LEU
1	A	14	ILE
1	A	18	ILE
1	A	20	VAL
1	A	22	GLN
1	A	25	PHE
1	A	29	LYS
1	A	30	VAL
1	A	32	HIS
1	A	34	SER
1	A	37	GLN
1	A	41	SER
1	A	42	PHE
1	A	47	THR
1	A	52	ARG
1	A	62	ASP
1	A	64	TYR
1	A	66	THR
1	A	67	PHE

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Mol	Chain	Res	Type
1	A	68	LEU
1	A	71	LEU
1	A	76	LEU
1	A	78	CYS
1	A	79	SER
1	A	89	MSE
1	A	90	TYR
1	A	91	LEU
1	A	94	ARG
1	A	95	GLN
1	A	96	LYS
1	A	99	VAL
1	A	101	TYR
1	A	108	SER
1	A	109	THR
1	A	112	TYR
1	A	114	PHE
1	A	117	ARG
1	A	118	ILE
1	A	119	ILE
1	A	121	PHE
1	A	122	LEU
1	A	124	LEU
1	A	130	ILE
1	A	131	PHE
1	A	132	ASN
1	A	133	TYR
1	A	135	LEU
1	B	1	MSE
1	B	8	ASN
1	B	11	LEU
1	B	14	ILE
1	B	18	ILE
1	B	20	VAL
1	B	21	VAL
1	B	22	GLN
1	B	25	PHE
1	B	29	LYS
1	B	30	VAL
1	B	32	HIS
1	B	34	SER
1	B	35	ARG

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Mol	Chain	Res	Type
1	B	37	GLN
1	B	50	PHE
1	B	52	ARG
1	B	62	ASP
1	B	66	THR
1	B	67	PHE
1	B	68	LEU
1	B	71	LEU
1	B	76	LEU
1	B	78	CYS
1	B	80	GLN
1	B	81	VAL
1	B	89	MSE
1	B	90	TYR
1	B	91	LEU
1	B	93	VAL
1	B	94	ARG
1	B	96	LYS
1	B	99	VAL
1	B	101	TYR
1	B	102	LEU
1	B	105	ARG
1	B	109	THR
1	B	113	ILE
1	B	114	PHE
1	B	117	ARG
1	B	118	ILE
1	B	119	ILE
1	B	121	PHE
1	B	122	LEU
1	B	124	LEU
1	B	130	ILE
1	B	131	PHE
1	B	132	ASN
1	B	133	TYR
1	B	135	LEU
1	B	142	ASP
1	B	143	PHE
1	B	144	GLU
1	B	145	ASN
1	B	146	TYR
1	C	1	MSE

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Mol	Chain	Res	Type
1	C	8	ASN
1	C	10	VAL
1	C	11	LEU
1	C	14	ILE
1	C	18	ILE
1	C	20	VAL
1	C	21	VAL
1	C	22	GLN
1	C	23	ASN
1	C	25	PHE
1	C	29	LYS
1	C	32	HIS
1	C	33	GLU
1	C	35	ARG
1	C	37	GLN
1	C	47	THR
1	C	52	ARG
1	C	62	ASP
1	C	64	TYR
1	C	66	THR
1	C	68	LEU
1	C	71	LEU
1	C	76	LEU
1	C	80	GLN
1	C	89	MSE
1	C	91	LEU
1	C	93	VAL
1	C	94	ARG
1	C	96	LYS
1	C	101	TYR
1	C	102	LEU
1	C	108	SER
1	C	118	ILE
1	C	119	ILE
1	C	122	LEU
1	C	124	LEU
1	C	130	ILE
1	C	131	PHE
1	C	132	ASN
1	C	133	TYR
1	C	141	SER
1	D	1	MSE

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Mol	Chain	Res	Type
1	D	8	ASN
1	D	10	VAL
1	D	11	LEU
1	D	14	ILE
1	D	18	ILE
1	D	20	VAL
1	D	21	VAL
1	D	22	GLN
1	D	29	LYS
1	D	30	VAL
1	D	32	HIS
1	D	35	ARG
1	D	41	SER
1	D	42	PHE
1	D	44	ARG
1	D	51	GLU
1	D	52	ARG
1	D	62	ASP
1	D	66	THR
1	D	67	PHE
1	D	68	LEU
1	D	71	LEU
1	D	76	LEU
1	D	79	SER
1	D	89	MSE
1	D	90	TYR
1	D	91	LEU
1	D	93	VAL
1	D	94	ARG
1	D	95	GLN
1	D	96	LYS
1	D	101	TYR
1	D	102	LEU
1	D	108	SER
1	D	113	ILE
1	D	114	PHE
1	D	116	LYS
1	D	118	ILE
1	D	119	ILE
1	D	122	LEU
1	D	124	LEU
1	D	125	MSE

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Mol	Chain	Res	Type
1	D	130	ILE
1	D	131	PHE
1	D	132	ASN
1	D	135	LEU
1	D	142	ASP
1	D	143	PHE
1	E	1	MSE
1	E	8	ASN
1	E	11	LEU
1	E	14	ILE
1	E	18	ILE
1	E	20	VAL
1	E	22	GLN
1	E	25	PHE
1	E	29	LYS
1	E	32	HIS
1	E	34	SER
1	E	35	ARG
1	E	37	GLN
1	E	40	ARG
1	E	42	PHE
1	E	44	ARG
1	E	45	THR
1	E	51	GLU
1	E	52	ARG
1	E	62	ASP
1	E	64	TYR
1	E	66	THR
1	E	67	PHE
1	E	68	LEU
1	E	71	LEU
1	E	76	LEU
1	E	80	GLN
1	E	81	VAL
1	E	89	MSE
1	E	90	TYR
1	E	91	LEU
1	E	94	ARG
1	E	96	LYS
1	E	99	VAL
1	E	101	TYR
1	E	102	LEU

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Mol	Chain	Res	Type
1	E	112	TYR
1	E	114	PHE
1	E	116	LYS
1	E	117	ARG
1	E	118	ILE
1	E	119	ILE
1	E	121	PHE
1	E	122	LEU
1	E	124	LEU
1	E	130	ILE
1	E	131	PHE
1	E	132	ASN
1	E	135	LEU
1	E	139	PHE
1	F	1	MSE
1	F	8	ASN
1	F	11	LEU
1	F	14	ILE
1	F	18	ILE
1	F	20	VAL
1	F	21	VAL
1	F	22	GLN
1	F	25	PHE
1	F	29	LYS
1	F	32	HIS
1	F	42	PHE
1	F	43	GLN
1	F	52	ARG
1	F	62	ASP
1	F	64	TYR
1	F	66	THR
1	F	67	PHE
1	F	68	LEU
1	F	71	LEU
1	F	76	LEU
1	F	78	CYS
1	F	81	VAL
1	F	89	MSE
1	F	90	TYR
1	F	91	LEU
1	F	93	VAL
1	F	94	ARG

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Mol	Chain	Res	Type
1	F	95	GLN
1	F	96	LYS
1	F	97	TYR
1	F	101	TYR
1	F	102	LEU
1	F	104	GLU
1	F	108	SER
1	F	109	THR
1	F	114	PHE
1	F	117	ARG
1	F	118	ILE
1	F	119	ILE
1	F	121	PHE
1	F	122	LEU
1	F	124	LEU
1	F	130	ILE
1	F	131	PHE
1	F	132	ASN
1	F	133	TYR
1	F	135	LEU
1	F	143	PHE
1	F	144	GLU
1	F	147	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	57	ASN
1	B	8	ASN
1	B	38	ASN
1	B	80	GLN
1	B	132	ASN
1	B	145	ASN
1	C	8	ASN
1	C	57	ASN
1	C	58	GLN
1	C	80	GLN
1	D	3	GLN
1	D	8	ASN
1	D	58	GLN
1	D	80	GLN

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Mol	Chain	Res	Type
1	D	95	GLN
1	E	8	ASN
1	E	37	GLN
1	E	59	ASN
1	E	80	GLN
1	E	132	ASN
1	F	8	ASN
1	F	43	GLN
1	F	80	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	3CS	B	502	-	40,47,47	2.02	17 (42%)	55,70,70	1.98	15 (27%)
2	3CS	E	506	-	40,47,47	1.94	12 (30%)	55,70,70	1.99	19 (34%)
2	3CS	D	505	-	40,47,47	2.09	15 (37%)	55,70,70	1.97	15 (27%)
2	3CS	A	503	-	40,47,47	2.16	16 (40%)	55,70,70	1.98	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	3CS	F	504	-	40,47,47	2.04	16 (40%)	55,70,70	1.98	16 (29%)
2	3CS	C	501	-	40,47,47	2.06	12 (30%)	55,70,70	1.97	14 (25%)

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	3CS	B	502	-	-	6/18/29/29	0/5/5/5
2	3CS	E	506	-	-	10/18/29/29	0/5/5/5
2	3CS	D	505	-	-	7/18/29/29	0/5/5/5
2	3CS	A	503	-	-	10/18/29/29	0/5/5/5
2	3CS	F	504	-	-	7/18/29/29	0/5/5/5
2	3CS	C	501	-	-	6/18/29/29	0/5/5/5

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	3CS	O27-C11	-6.06	1.23	1.37
2	A	503	3CS	C40-C41	-5.64	1.41	1.50
2	C	501	3CS	C30-C29	-5.51	1.45	1.51
2	D	505	3CS	C30-C29	-5.29	1.45	1.51
2	F	504	3CS	O27-C11	-5.08	1.25	1.37
2	E	506	3CS	O27-C11	-5.06	1.25	1.37
2	A	503	3CS	O27-C11	-4.75	1.26	1.37
2	D	505	3CS	O27-C11	-4.70	1.26	1.37
2	B	502	3CS	O27-C11	-4.61	1.27	1.37
2	F	504	3CS	C30-C29	-4.50	1.46	1.51
2	E	506	3CS	C30-C29	-4.37	1.46	1.51
2	B	502	3CS	C30-C29	-4.24	1.46	1.51
2	A	503	3CS	C30-C29	-3.90	1.47	1.51
2	F	504	3CS	C40-C41	-3.75	1.44	1.50
2	B	502	3CS	C12-C11	3.68	1.43	1.37
2	C	501	3CS	O27-C10	-3.58	1.31	1.43
2	D	505	3CS	C18-N17	-3.50	1.42	1.48
2	C	501	3CS	C40-C41	-3.33	1.45	1.50
2	F	504	3CS	C23-C22	3.33	1.44	1.38
2	A	503	3CS	C12-C11	3.25	1.42	1.37
2	D	505	3CS	C40-C41	-3.24	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	503	3CS	C9-N26	3.23	1.38	1.32
2	A	503	3CS	C24-I25	-3.20	2.02	2.10
2	E	506	3CS	C12-C11	3.17	1.42	1.37
2	C	501	3CS	C18-C19	-3.04	1.44	1.51
2	E	506	3CS	O27-C10	-3.00	1.33	1.43
2	F	504	3CS	C12-C11	2.90	1.42	1.37
2	D	505	3CS	C12-C11	2.89	1.42	1.37
2	D	505	3CS	O27-C10	-2.87	1.34	1.43
2	D	505	3CS	C14-C13	2.84	1.42	1.36
2	F	504	3CS	C22-C24	2.84	1.45	1.38
2	E	506	3CS	C18-N17	-2.82	1.43	1.48
2	D	505	3CS	C18-C19	-2.80	1.44	1.51
2	B	502	3CS	C4-C5	2.75	1.43	1.36
2	B	502	3CS	O27-C10	-2.74	1.34	1.43
2	C	501	3CS	C10-C9	-2.73	1.43	1.50
2	A	503	3CS	C1-C6	2.73	1.46	1.42
2	A	503	3CS	C18-N17	-2.73	1.43	1.48
2	A	503	3CS	O27-C10	-2.73	1.34	1.43
2	F	504	3CS	O27-C10	-2.71	1.34	1.43
2	D	505	3CS	C9-N26	2.71	1.37	1.32
2	B	502	3CS	C9-N26	2.69	1.37	1.32
2	C	501	3CS	C12-C11	2.67	1.41	1.37
2	B	502	3CS	C1-C6	2.64	1.46	1.42
2	A	503	3CS	C3-C2	2.61	1.42	1.36
2	F	504	3CS	C9-N26	2.58	1.37	1.32
2	B	502	3CS	C18-C19	-2.57	1.45	1.51
2	B	502	3CS	C3-C2	2.55	1.42	1.36
2	E	506	3CS	C4-C5	2.55	1.42	1.36
2	A	503	3CS	C4-C5	2.54	1.42	1.36
2	B	502	3CS	C18-N17	-2.54	1.43	1.48
2	C	501	3CS	C18-N17	-2.49	1.44	1.48
2	C	501	3CS	C24-I25	-2.44	2.04	2.10
2	D	505	3CS	C10-C9	-2.43	1.44	1.50
2	F	504	3CS	C4-C5	2.43	1.42	1.36
2	E	506	3CS	C3-C2	2.42	1.42	1.36
2	B	502	3CS	C14-C13	2.42	1.41	1.36
2	E	506	3CS	C1-C6	2.40	1.45	1.42
2	A	503	3CS	C18-C19	-2.38	1.45	1.51
2	A	503	3CS	C37-C36	-2.37	1.46	1.50
2	C	501	3CS	C4-C5	2.34	1.42	1.36
2	D	505	3CS	C4-C5	2.33	1.42	1.36
2	E	506	3CS	C10-C9	-2.32	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	506	3CS	C13-C11	2.29	1.43	1.38
2	D	505	3CS	C3-C2	2.29	1.41	1.36
2	B	502	3CS	C40-C41	-2.29	1.47	1.50
2	A	503	3CS	C14-C13	2.29	1.41	1.36
2	F	504	3CS	C21-C24	2.28	1.43	1.38
2	A	503	3CS	C7-C8	2.28	1.41	1.36
2	F	504	3CS	C3-C2	2.28	1.41	1.36
2	B	502	3CS	C24-I25	-2.27	2.04	2.10
2	F	504	3CS	C18-C19	-2.27	1.45	1.51
2	C	501	3CS	C3-C2	2.26	1.41	1.36
2	B	502	3CS	C13-C11	2.24	1.43	1.38
2	F	504	3CS	C21-C20	2.23	1.42	1.38
2	B	502	3CS	C7-C8	2.19	1.41	1.36
2	A	503	3CS	C10-C9	-2.17	1.45	1.50
2	E	506	3CS	C14-C13	2.15	1.41	1.36
2	F	504	3CS	C18-N17	-2.13	1.44	1.48
2	D	505	3CS	C7-C8	2.13	1.41	1.36
2	E	506	3CS	C4-C3	2.10	1.43	1.38
2	D	505	3CS	C13-C11	2.09	1.42	1.38
2	F	504	3CS	C14-C13	2.09	1.41	1.36
2	C	501	3CS	C6-N26	-2.07	1.34	1.37
2	B	502	3CS	C10-C9	-2.07	1.45	1.50
2	B	502	3CS	C23-C22	2.07	1.42	1.38
2	D	505	3CS	C23-C22	2.03	1.42	1.38
2	F	504	3CS	C23-C19	2.00	1.43	1.38

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	505	3CS	O35-C29-C30	-7.24	110.88	120.62
2	C	501	3CS	O35-C29-C30	-7.19	110.95	120.62
2	B	502	3CS	O35-C29-C30	-6.54	111.83	120.62
2	F	504	3CS	O35-C29-C30	-6.42	111.99	120.62
2	E	506	3CS	O35-C29-C30	-6.02	112.53	120.62
2	A	503	3CS	O35-C29-C30	-5.95	112.62	120.62
2	F	504	3CS	C37-C36-C28	-5.64	120.72	130.34
2	B	502	3CS	C37-C36-C28	-4.79	122.17	130.34
2	D	505	3CS	C37-C36-C28	-4.55	122.58	130.34
2	C	501	3CS	C37-C36-C28	-4.43	122.78	130.34
2	B	502	3CS	C10-O27-C11	4.35	128.40	117.65
2	E	506	3CS	C37-C36-C28	-4.29	123.03	130.34
2	A	503	3CS	C10-O27-C11	3.82	127.09	117.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	503	3CS	C37-C36-C28	-3.81	123.83	130.34
2	B	502	3CS	C33-C30-C29	3.60	123.71	117.06
2	E	506	3CS	C22-C24-I25	-3.46	114.47	119.68
2	A	503	3CS	C33-C30-C29	3.41	123.35	117.06
2	A	503	3CS	C36-C28-C16	-3.36	102.59	108.82
2	C	501	3CS	O27-C11-C12	-3.35	112.64	123.96
2	D	505	3CS	O27-C11-C12	-3.35	112.65	123.96
2	D	505	3CS	C10-O27-C11	3.33	125.88	117.65
2	C	501	3CS	C36-C28-C16	-3.31	102.69	108.82
2	D	505	3CS	C1-C6-N26	-3.30	117.35	122.26
2	E	506	3CS	O27-C11-C12	-3.26	112.94	123.96
2	D	505	3CS	C36-C28-C16	-3.24	102.82	108.82
2	C	501	3CS	C1-C6-N26	-3.22	117.47	122.26
2	B	502	3CS	O27-C11-C12	-3.21	113.10	123.96
2	E	506	3CS	C4-C5-C6	-3.21	115.46	120.08
2	A	503	3CS	O27-C11-C12	-3.19	113.17	123.96
2	A	503	3CS	C1-C6-N26	-3.18	117.53	122.26
2	F	504	3CS	C10-O27-C11	3.17	125.48	117.65
2	E	506	3CS	C5-C6-C1	3.16	122.36	119.04
2	A	503	3CS	C5-C6-C1	3.15	122.36	119.04
2	C	501	3CS	C5-C6-C1	3.10	122.30	119.04
2	B	502	3CS	C36-C28-C16	-3.09	103.08	108.82
2	F	504	3CS	O27-C11-C12	-3.07	113.57	123.96
2	F	504	3CS	C33-C30-C29	3.06	122.71	117.06
2	E	506	3CS	C10-O27-C11	2.92	124.87	117.65
2	F	504	3CS	C36-C28-C16	-2.91	103.42	108.82
2	F	504	3CS	O27-C10-C9	2.91	117.25	109.42
2	A	503	3CS	C22-C24-C21	2.89	124.67	120.63
2	D	505	3CS	C34-C33-C30	2.89	119.28	109.71
2	D	505	3CS	C5-C6-C1	2.87	122.06	119.04
2	A	503	3CS	C21-C24-I25	-2.84	115.39	119.68
2	B	502	3CS	C4-C5-C6	-2.78	116.08	120.08
2	E	506	3CS	C11-C12-C16	-2.76	116.38	120.05
2	A	503	3CS	C4-C5-C6	-2.73	116.15	120.08
2	B	502	3CS	C1-C6-N26	-2.73	118.20	122.26
2	F	504	3CS	C1-C6-N26	-2.71	118.23	122.26
2	D	505	3CS	C4-C5-C6	-2.70	116.19	120.08
2	E	506	3CS	C3-C2-C1	-2.67	116.27	120.44
2	F	504	3CS	C34-C33-C30	2.66	118.53	109.71
2	C	501	3CS	C4-C5-C6	-2.66	116.26	120.08
2	D	505	3CS	C38-C40-C41	-2.60	103.04	109.45
2	E	506	3CS	C36-C28-C16	-2.60	104.00	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	506	3CS	C34-C33-C30	2.58	118.23	109.71
2	E	506	3CS	C39-C40-C38	-2.57	100.24	107.28
2	B	502	3CS	C34-C33-C30	2.57	118.21	109.71
2	C	501	3CS	C13-C11-C12	2.56	124.25	120.81
2	B	502	3CS	C3-C2-C1	-2.55	116.45	120.44
2	E	506	3CS	C33-C30-C29	2.54	121.75	117.06
2	E	506	3CS	C1-C6-N26	-2.54	118.49	122.26
2	F	504	3CS	O35-C29-C28	2.52	124.76	120.12
2	D	505	3CS	C7-C8-C9	-2.52	116.15	119.18
2	E	506	3CS	C7-C1-C2	-2.48	117.39	123.19
2	E	506	3CS	O27-C10-C9	2.42	115.93	109.42
2	C	501	3CS	C33-C30-C29	2.40	121.48	117.06
2	C	501	3CS	C7-C1-C2	-2.40	117.59	123.19
2	C	501	3CS	C22-C24-C21	2.36	123.92	120.63
2	F	504	3CS	C4-C5-C6	-2.35	116.70	120.08
2	D	505	3CS	C33-C30-C29	2.35	121.39	117.06
2	B	502	3CS	O27-C10-C9	2.34	115.73	109.42
2	C	501	3CS	O35-C29-C28	2.34	124.42	120.12
2	F	504	3CS	C11-C12-C16	-2.31	116.97	120.05
2	B	502	3CS	C5-C6-C1	2.31	121.47	119.04
2	D	505	3CS	C9-N26-C6	2.30	121.86	118.00
2	F	504	3CS	C22-C24-I25	2.28	123.12	119.68
2	E	506	3CS	C21-C24-I25	2.25	123.07	119.68
2	F	504	3CS	C7-C1-C2	-2.24	117.95	123.19
2	B	502	3CS	C7-C1-C2	-2.23	117.98	123.19
2	B	502	3CS	C2-C1-C6	2.22	121.58	118.45
2	C	501	3CS	C7-C1-C6	2.21	121.57	118.45
2	A	503	3CS	C34-C33-C30	2.20	116.99	109.71
2	A	503	3CS	C3-C2-C1	-2.20	117.01	120.44
2	D	505	3CS	C3-C2-C1	-2.19	117.02	120.44
2	F	504	3CS	C5-C6-C1	2.19	121.34	119.04
2	B	502	3CS	O35-C29-C28	2.18	124.12	120.12
2	E	506	3CS	C13-C14-C15	-2.15	116.40	119.70
2	A	503	3CS	C7-C1-C6	2.11	121.44	118.45
2	A	503	3CS	C20-C21-C24	-2.11	116.78	119.56
2	A	503	3CS	C7-C1-C2	-2.10	118.28	123.19
2	A	503	3CS	C23-C22-C24	-2.09	116.81	119.56
2	C	501	3CS	C20-C21-C24	-2.09	116.81	119.56
2	E	506	3CS	C2-C1-C6	2.06	121.36	118.45
2	F	504	3CS	C13-C14-C15	-2.04	116.56	119.70
2	D	505	3CS	C7-C1-C2	-2.02	118.47	123.19

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	3CS	C36-C37-C40-C38
2	A	503	3CS	C36-C37-C40-C39
2	A	503	3CS	C36-C37-C40-C41
2	B	502	3CS	C36-C37-C40-C38
2	B	502	3CS	C36-C37-C40-C39
2	B	502	3CS	C36-C37-C40-C41
2	C	501	3CS	C19-C18-N17-C36
2	E	506	3CS	C29-C30-C33-C31
2	E	506	3CS	C29-C30-C33-C32
2	E	506	3CS	C29-C30-C33-C34
2	F	504	3CS	C19-C18-N17-C36
2	F	504	3CS	C36-C37-C40-C38
2	F	504	3CS	C36-C37-C40-C39
2	F	504	3CS	C36-C37-C40-C41
2	C	501	3CS	C12-C11-O27-C10
2	C	501	3CS	C13-C11-O27-C10
2	F	504	3CS	C12-C11-O27-C10
2	F	504	3CS	C13-C11-O27-C10
2	E	506	3CS	C12-C11-O27-C10
2	E	506	3CS	C13-C11-O27-C10
2	C	501	3CS	C29-C30-C33-C31
2	C	501	3CS	C29-C30-C33-C32
2	D	505	3CS	C12-C11-O27-C10
2	D	505	3CS	C13-C11-O27-C10
2	A	503	3CS	C12-C11-O27-C10
2	E	506	3CS	O35-C29-C30-C33
2	E	506	3CS	C28-C29-C30-C33
2	A	503	3CS	C13-C11-O27-C10
2	A	503	3CS	C19-C18-N17-C36
2	B	502	3CS	C19-C18-N17-C36
2	D	505	3CS	C19-C18-N17-C36
2	E	506	3CS	C19-C18-N17-C36
2	C	501	3CS	C29-C30-C33-C34
2	D	505	3CS	O27-C10-C9-N26
2	D	505	3CS	C28-C29-C30-C33
2	A	503	3CS	O27-C10-C9-N26
2	B	502	3CS	O27-C10-C9-N26
2	D	505	3CS	O27-C10-C9-C8
2	E	506	3CS	N17-C18-C19-C20
2	B	502	3CS	O27-C10-C9-C8
2	E	506	3CS	N17-C18-C19-C23
2	A	503	3CS	N17-C36-C37-C40

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Mol	Chain	Res	Type	Atoms
2	A	503	3CS	O27-C10-C9-C8
2	A	503	3CS	N17-C18-C19-C20
2	D	505	3CS	O35-C29-C30-C33
2	F	504	3CS	O35-C29-C30-C33

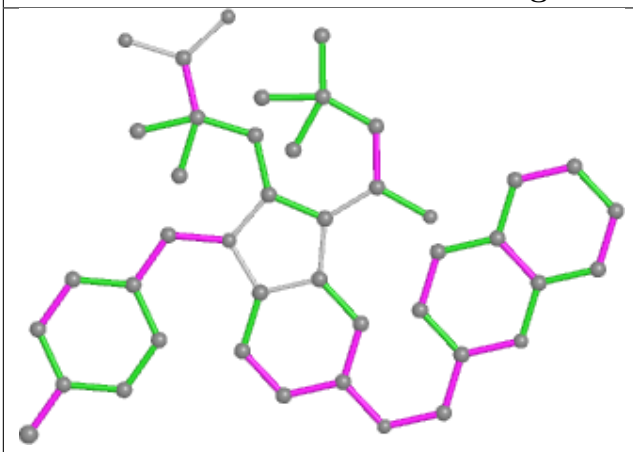
There are no ring outliers.

6 monomers are involved in 141 short contacts:

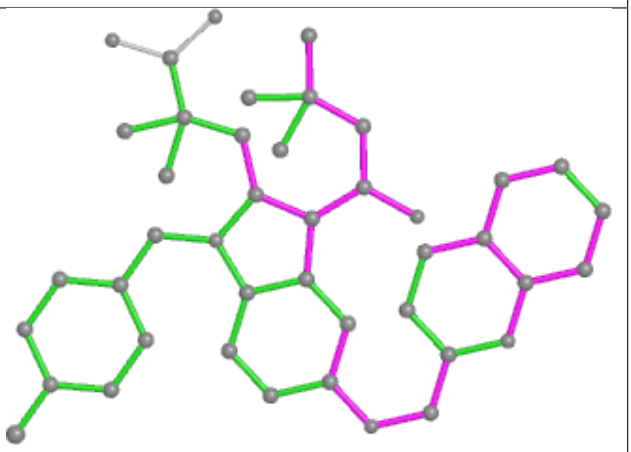
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	3CS	19	0
2	E	506	3CS	23	0
2	D	505	3CS	28	0
2	A	503	3CS	29	0
2	F	504	3CS	21	0
2	C	501	3CS	21	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

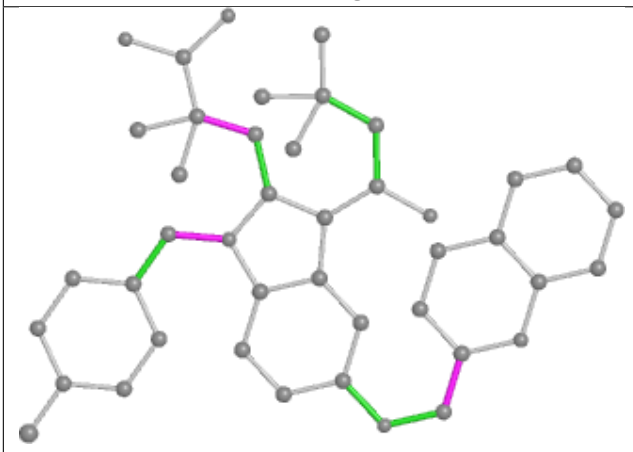
Ligand 3CS B 502



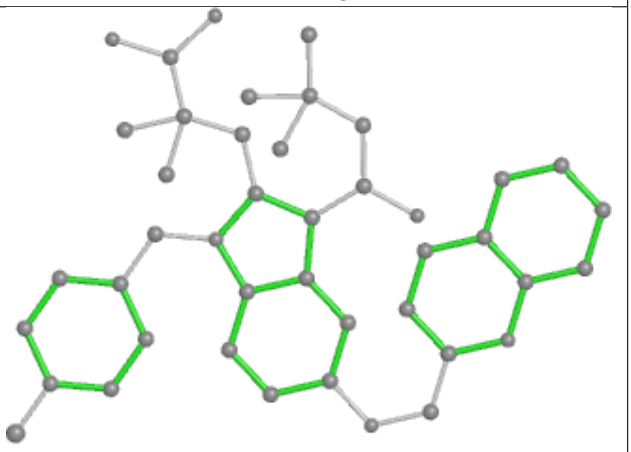
Bond lengths



Bond angles

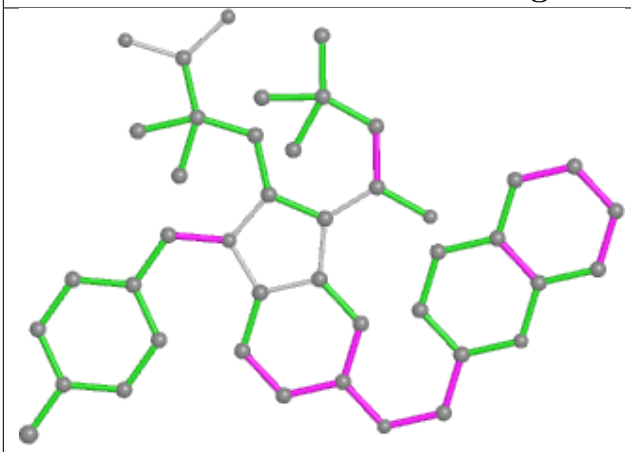


Torsions

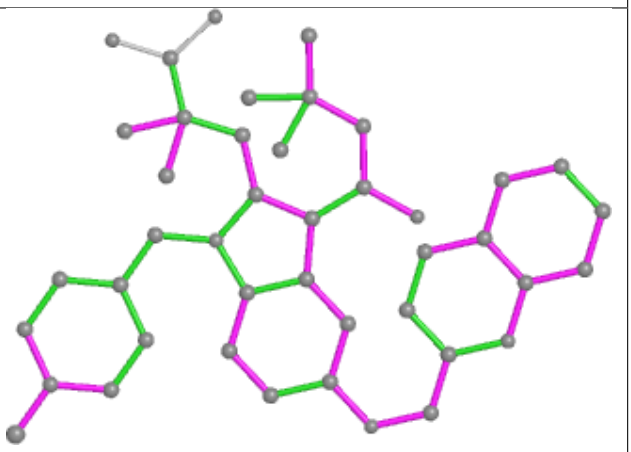


Rings

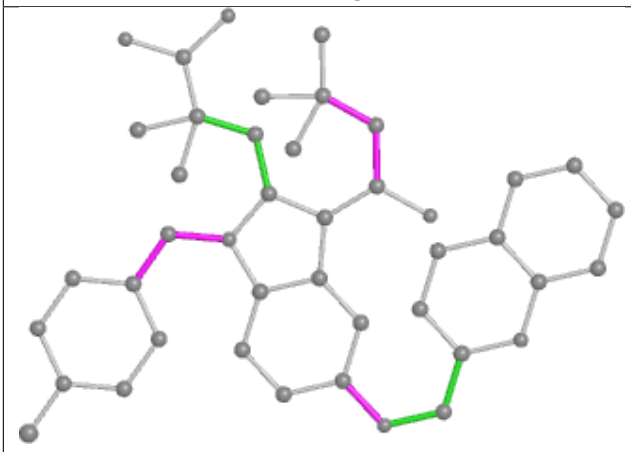
Ligand 3CS E 506



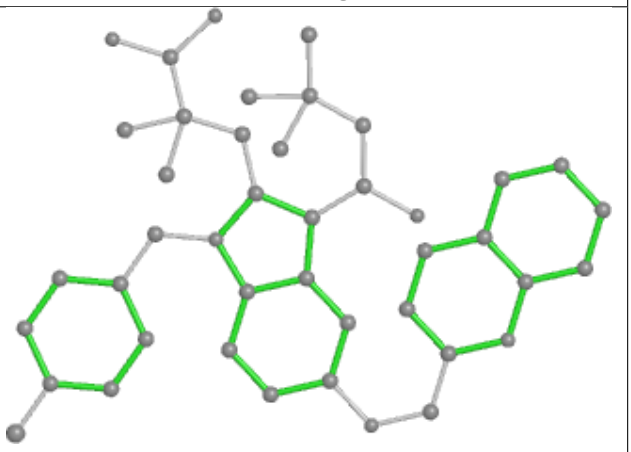
Bond lengths



Bond angles

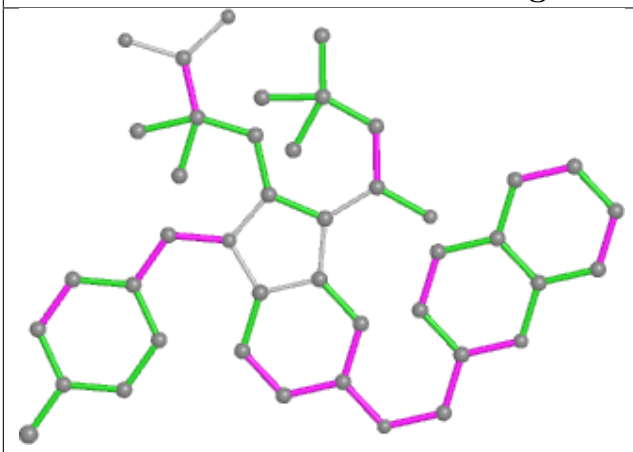


Torsions

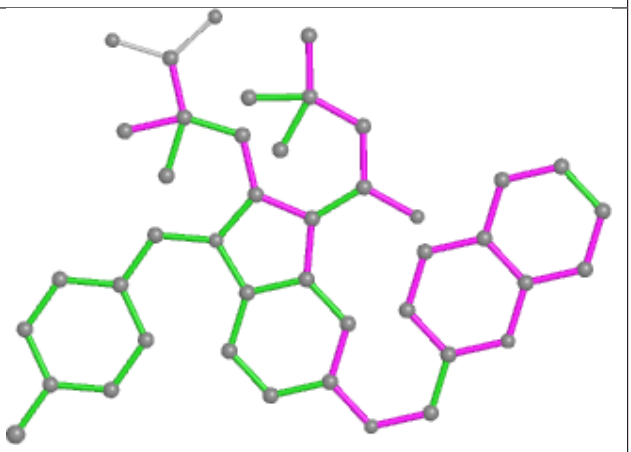


Rings

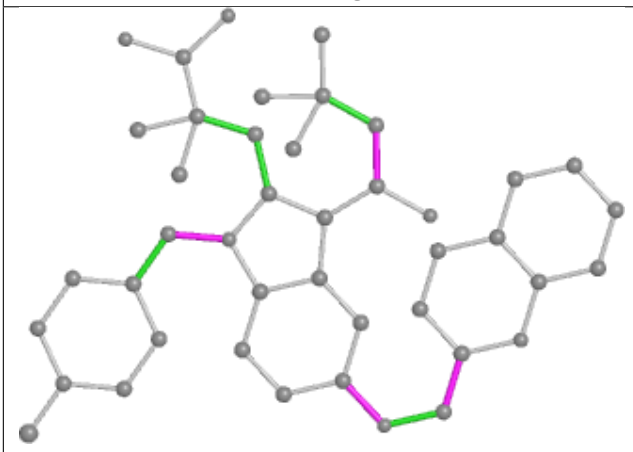
Ligand 3CS D 505



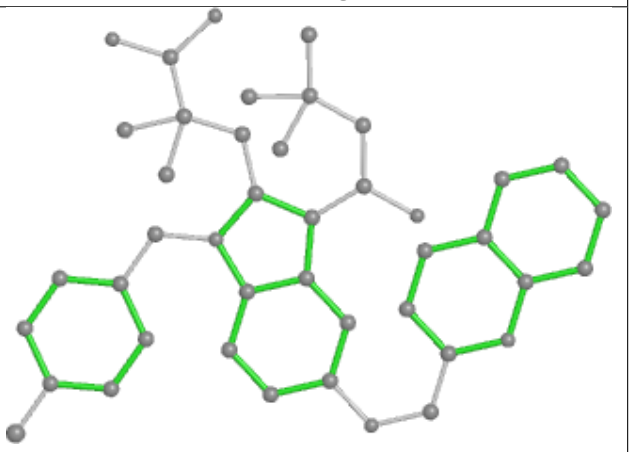
Bond lengths



Bond angles

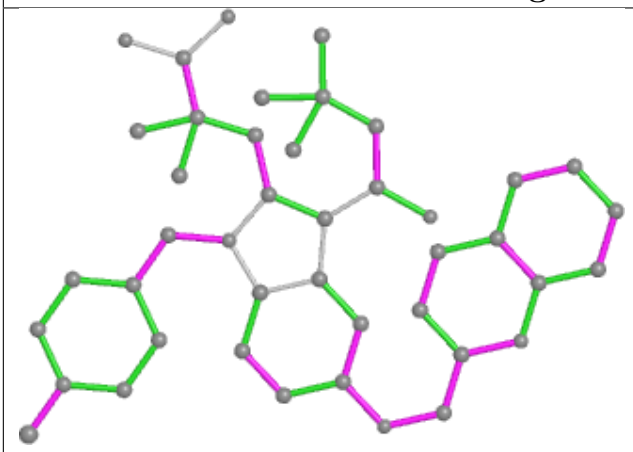


Torsions

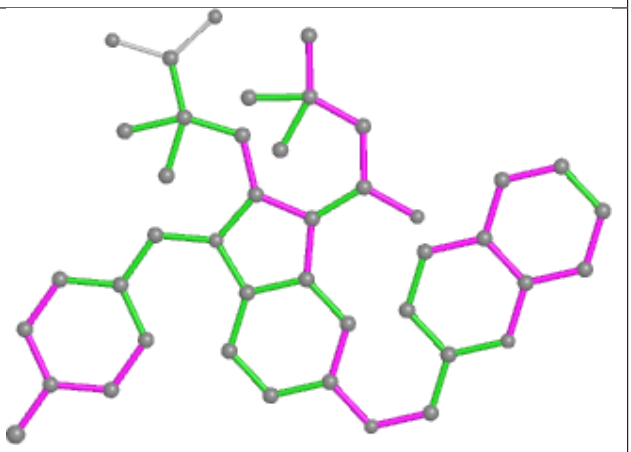


Rings

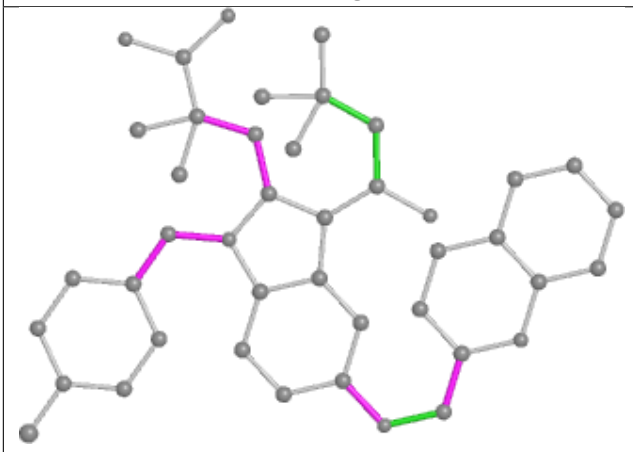
Ligand 3CS A 503



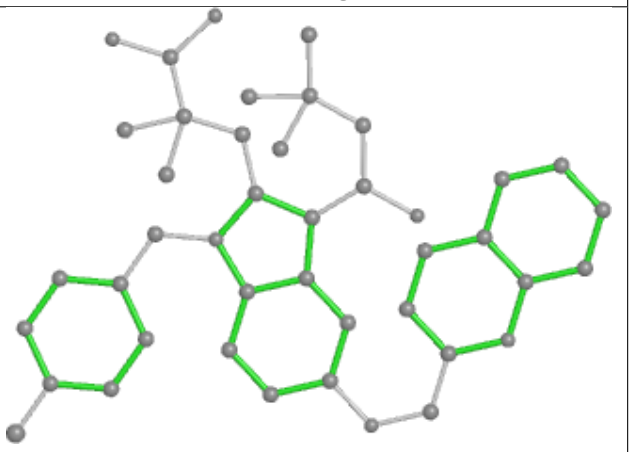
Bond lengths



Bond angles

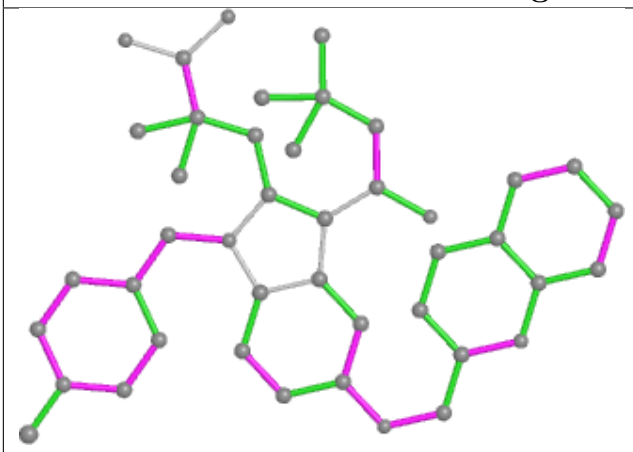


Torsions

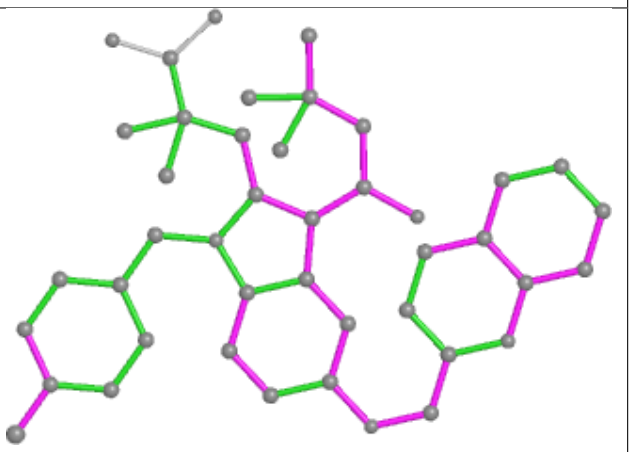


Rings

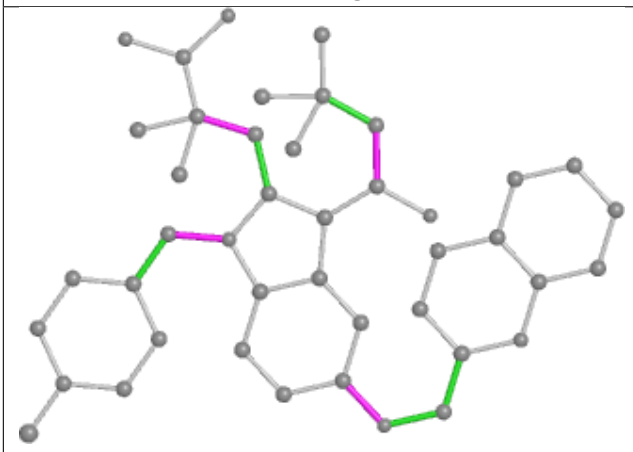
Ligand 3CS F 504



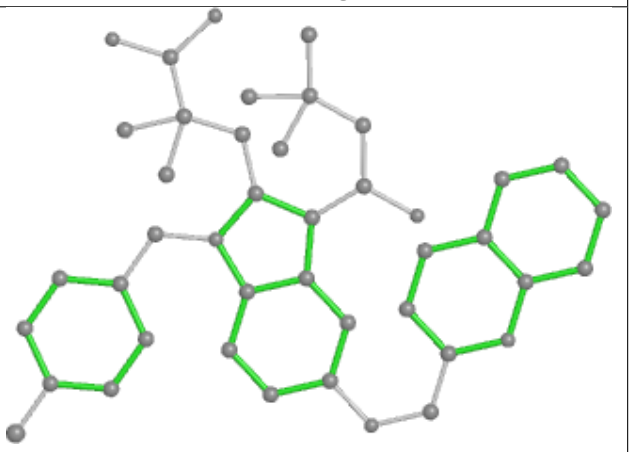
Bond lengths



Bond angles

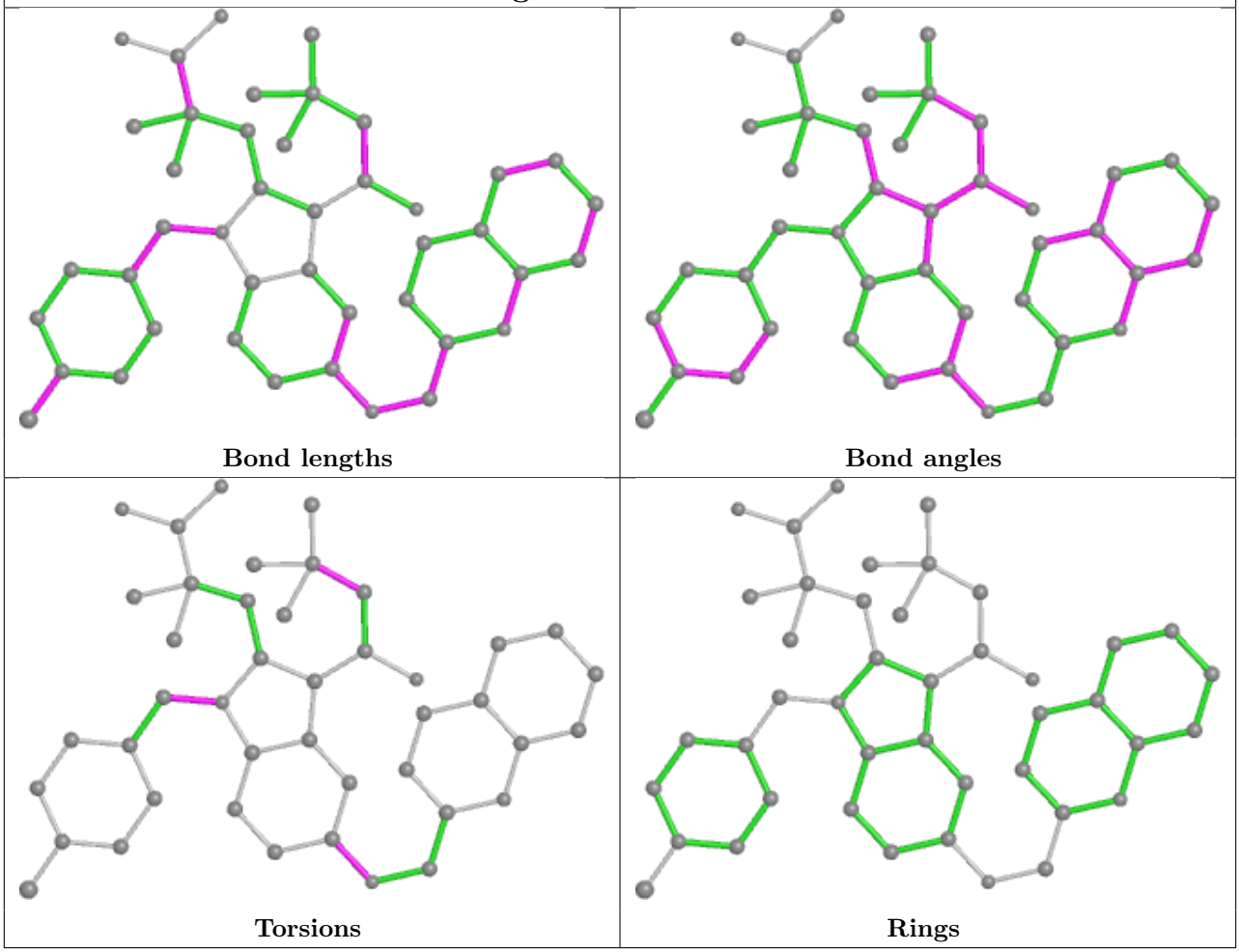


Torsions



Rings

Ligand 3CS C 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	137/161 (85%)	-0.22	1 (0%)	87	82	78, 114, 163, 182	0
1	B	145/161 (90%)	-0.41	0	100	100	75, 112, 162, 171	0
1	C	146/161 (90%)	-0.32	0	100	100	67, 105, 158, 173	0
1	D	145/161 (90%)	-0.38	1 (0%)	87	82	74, 114, 163, 170	0
1	E	137/161 (85%)	-0.25	2 (1%)	73	64	83, 117, 170, 188	0
1	F	146/161 (90%)	-0.16	3 (2%)	63	54	80, 117, 172, 205	0
All	All	856/966 (88%)	-0.29	7 (0%)	86	79	67, 114, 165, 205	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	43	GLN	4.4
1	F	44	ARG	4.1
1	E	107	GLN	3.3
1	A	140	GLY	2.6
1	D	45	THR	2.5
1	E	140	GLY	2.3
1	F	149	THR	2.3

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 monosaccharides in this entry.

6.4 Ligands (i)

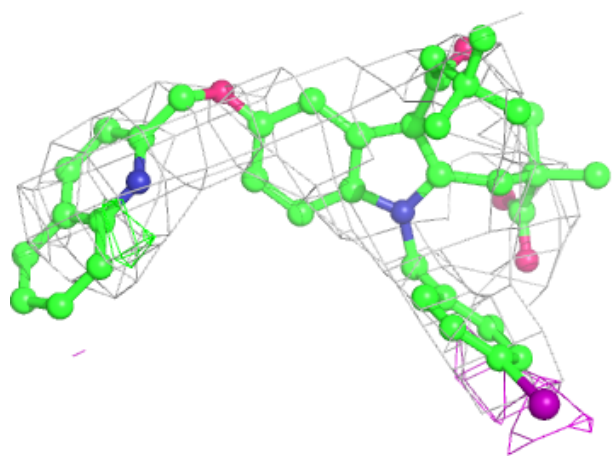
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

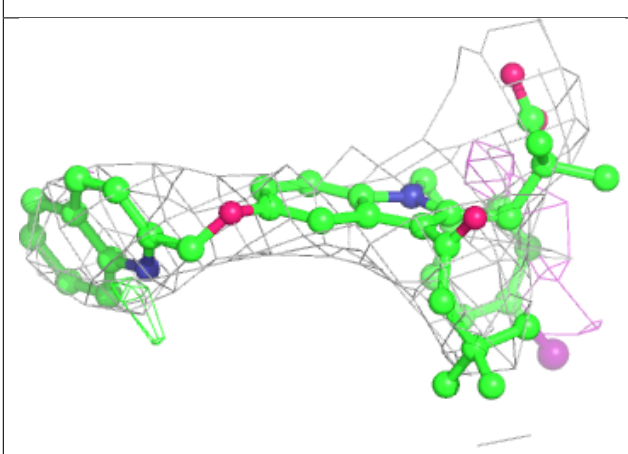
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	3CS	E	506	43/43	0.88	0.41	160,160,160,160	0
2	3CS	F	504	43/43	0.88	0.36	155,155,155,155	0
2	3CS	D	505	43/43	0.90	0.34	159,159,159,159	0
2	3CS	A	503	43/43	0.91	0.31	159,159,159,159	0
2	3CS	B	502	43/43	0.91	0.41	152,152,152,152	0
2	3CS	C	501	43/43	0.91	0.33	155,155,155,155	0

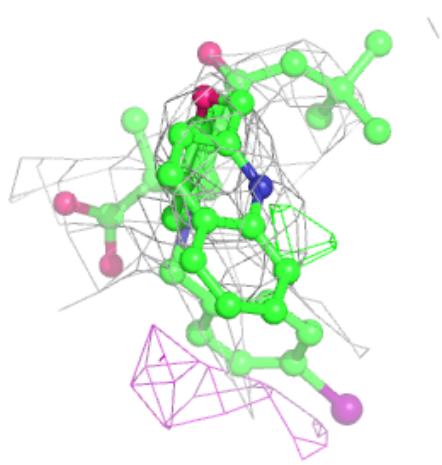
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 3CS E 506:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

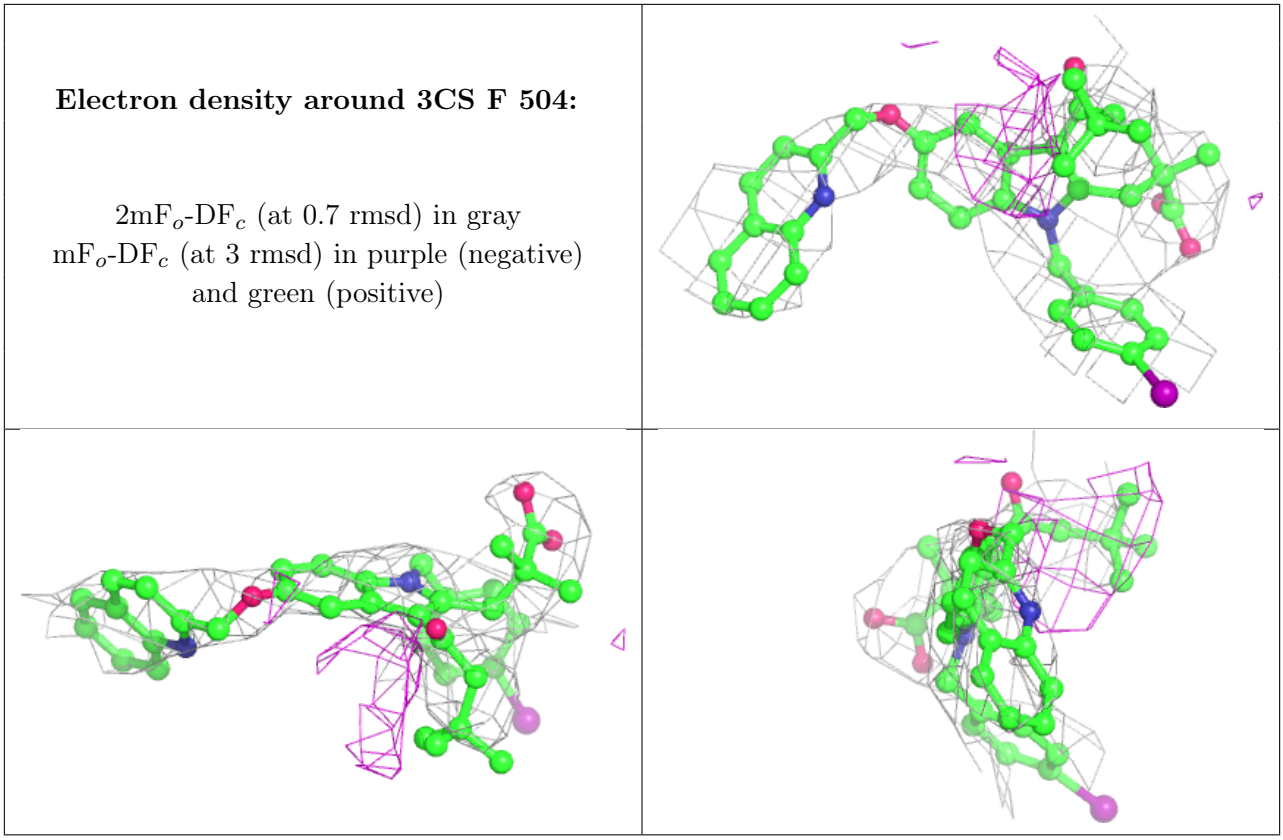






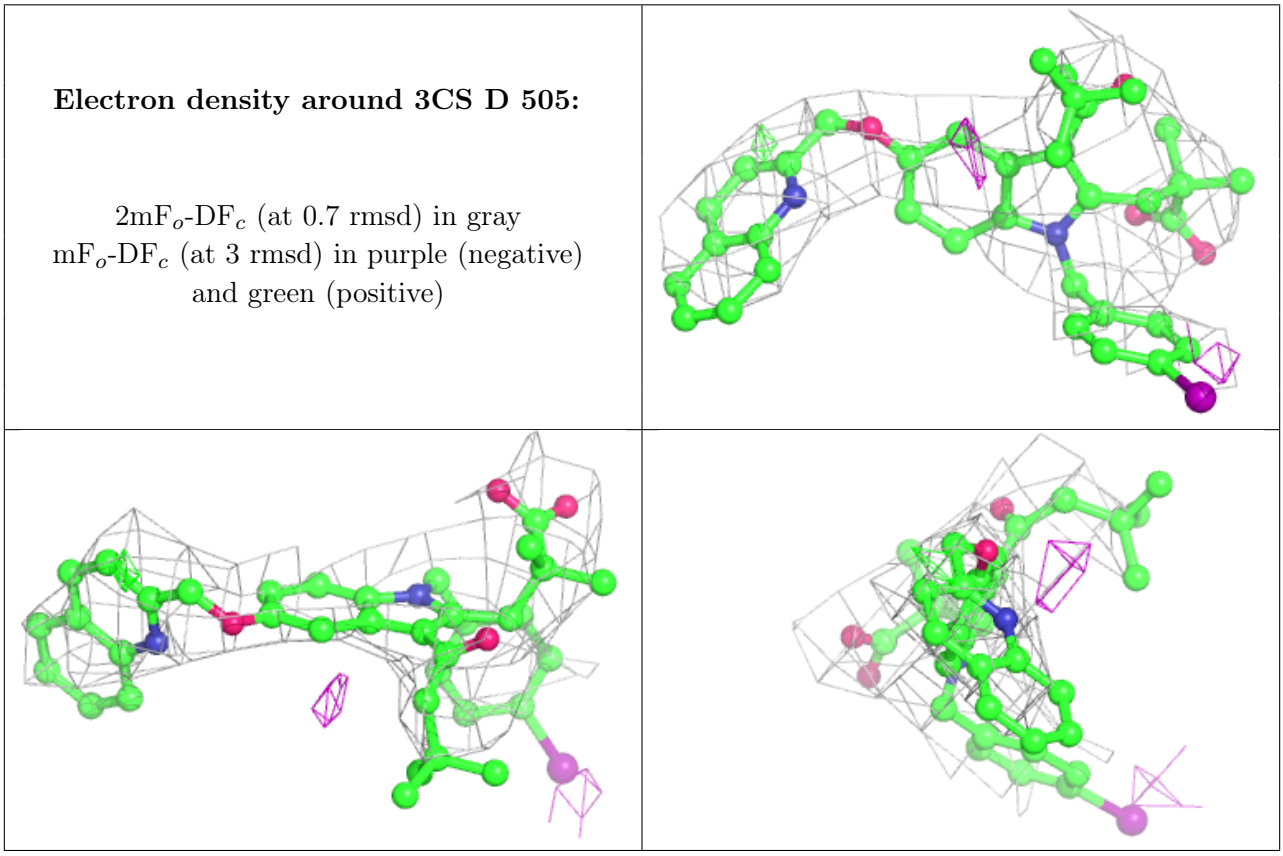
Electron density around 3CS F 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



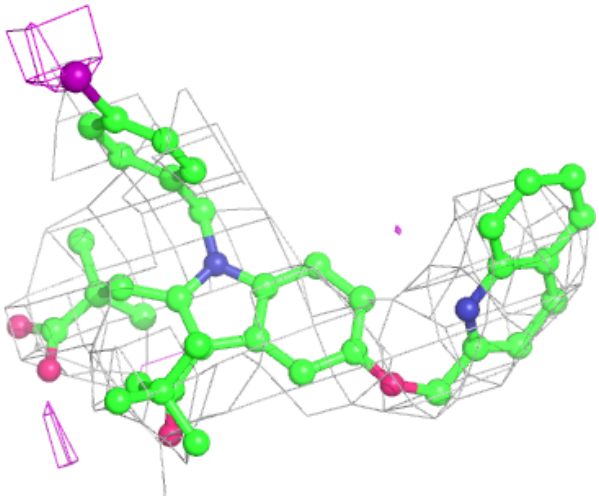
Electron density around 3CS D 505:

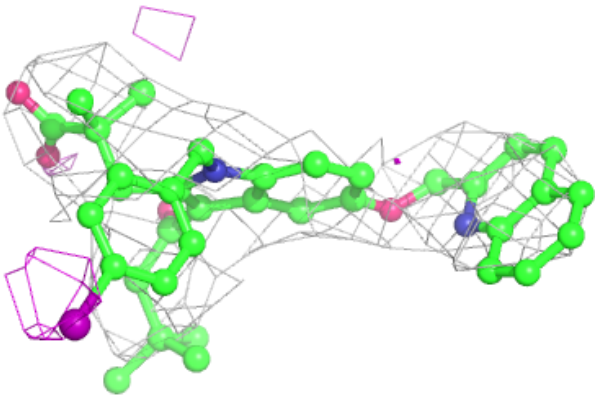
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

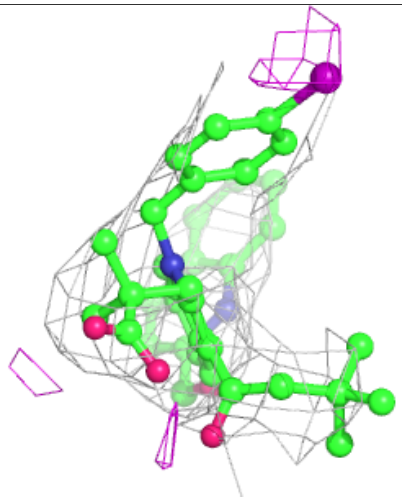


Electron density around 3CS A 503:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

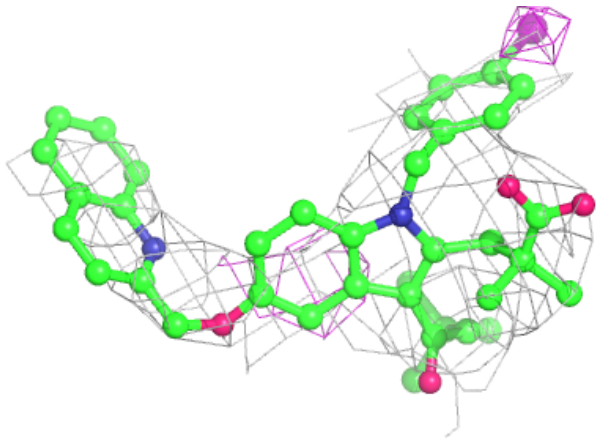


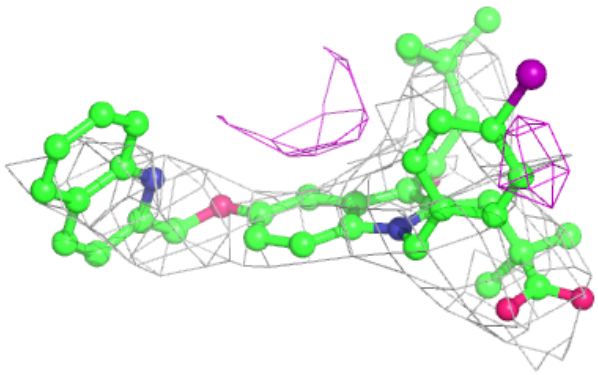


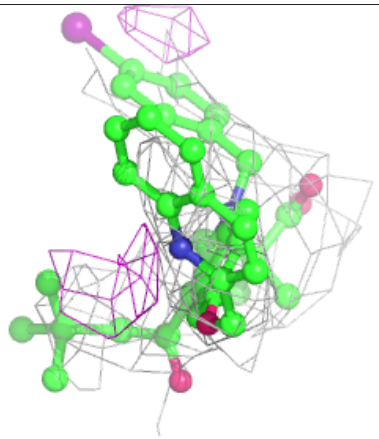


Electron density around 3CS B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

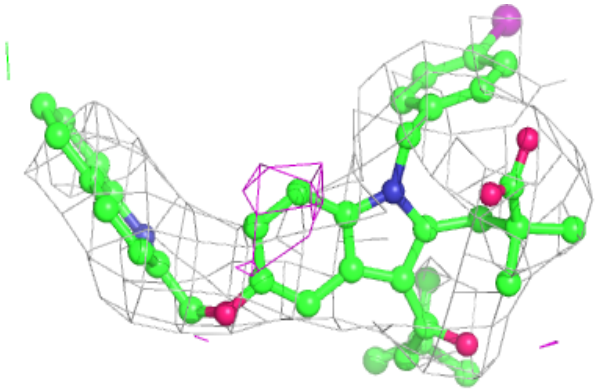


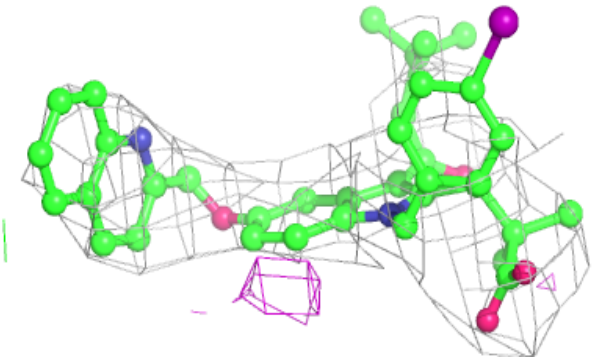


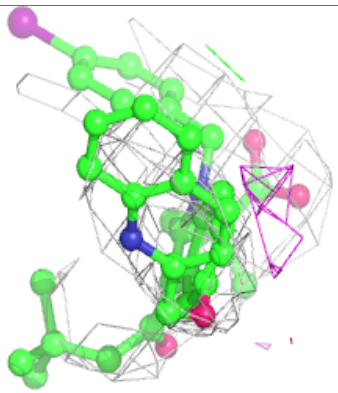


Electron density around 3CS C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.