



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:20 am BST

PDB ID : 1XLS
Title : Crystal structure of the mouse CAR/RXR LBD heterodimer bound to TCPOBOP and 9cRA and a TIF2 peptide containing the third LXXLL motifs
Authors : Suino, K.; peng, L.; Reynolds, R.; Li, Y.; Cha, J.-Y.; Repa, J.J.; Kliewer, S.A.; Xu, H.E.
Deposited on : 2004-09-30
Resolution : 2.96 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

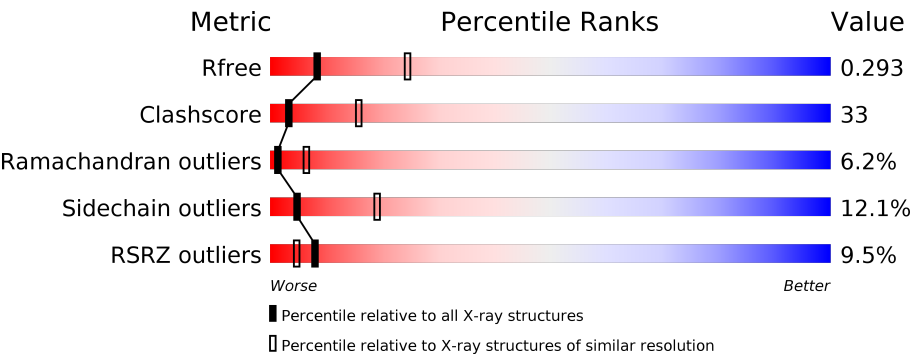
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	<div><div>10%</div><div><div></div><div>56%</div><div>35%</div><div>8%</div></div></div>
1	B	232	<div><div>11%</div><div><div></div><div>55%</div><div>37%</div><div>8%</div></div></div>
1	C	232	<div><div>11%</div><div><div></div><div>57%</div><div>34%</div><div>9%</div></div></div>
1	D	232	<div><div>9%</div><div><div></div><div>56%</div><div>34%</div><div>9%</div></div></div>
2	E	242	<div><div>5%</div><div><div></div><div>44%</div><div>43%</div><div>10%</div><div></div></div></div>
2	F	242	<div><div>5%</div><div><div></div><div>47%</div><div>42%</div><div>9%</div><div></div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	242	
2	H	242	
3	I	18	
3	J	18	
3	K	18	
3	L	18	
3	M	18	
3	N	18	
3	O	18	
3	P	18	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16288 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1755	1117	306	322	10			
1	B	232	Total	C	N	O	S	0	0	0
			1755	1117	306	322	10			
1	C	232	Total	C	N	O	S	0	0	0
			1755	1117	306	322	10			
1	D	232	Total	C	N	O	S	0	0	0
			1755	1117	306	322	10			

- Molecule 2 is a protein called Orphan nuclear receptor NR1I3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	242	Total	C	N	O	S	0	0	0
			1969	1269	334	353	13			
2	F	242	Total	C	N	O	S	0	0	0
			1969	1269	334	353	13			
2	G	242	Total	C	N	O	S	0	0	0
			1969	1269	334	353	13			
2	H	242	Total	C	N	O	S	0	0	0
			1969	1269	334	353	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	146	ARG	LYS	CONFLICT	UNP O35627
F	146	ARG	LYS	CONFLICT	UNP O35627
G	146	ARG	LYS	CONFLICT	UNP O35627
H	146	ARG	LYS	CONFLICT	UNP O35627

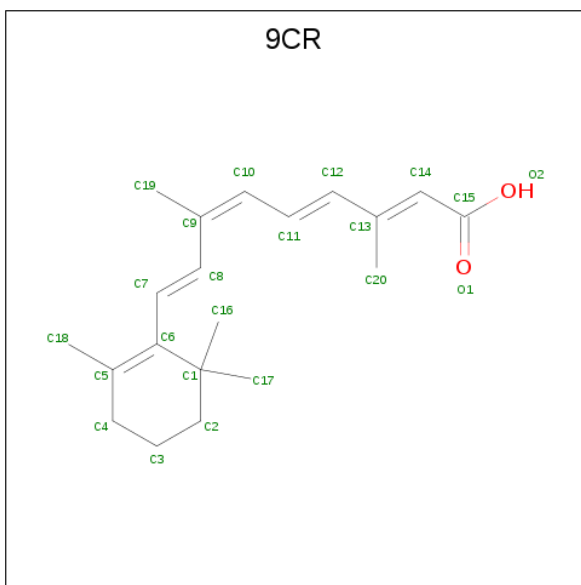
- Molecule 3 is a protein called Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	16	Total	C	N	O	0	0	0
			131	82	22	27			
3	J	16	Total	C	N	O	0	0	0
			131	82	22	27			
3	K	16	Total	C	N	O	0	0	0
			131	82	22	27			
3	L	16	Total	C	N	O	0	0	0
			131	82	22	27			
3	M	18	Total	C	N	O	0	0	0
			149	92	25	32			
3	N	18	Total	C	N	O	0	0	0
			149	92	25	32			
3	O	18	Total	C	N	O	0	0	0
			149	92	25	32			
3	P	18	Total	C	N	O	0	0	0
			149	92	25	32			

There are 8 discrepancies between the modelled and reference sequences:

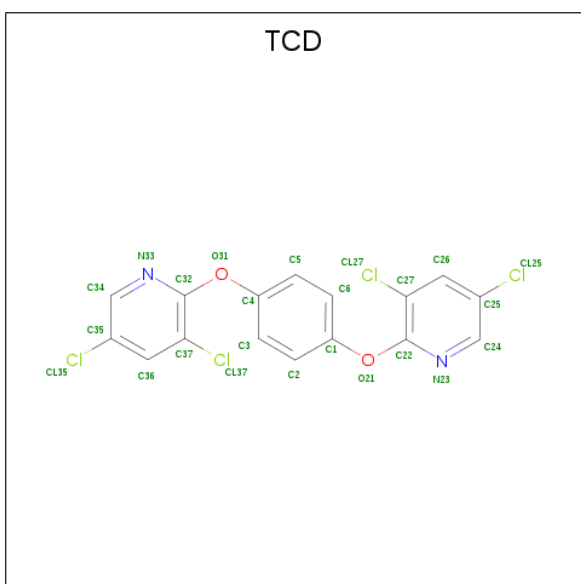
Chain	Residue	Modelled	Actual	Comment	Reference
I	739	ALA	LYS	CONFLICT	UNP Q9WUI9
J	739	ALA	LYS	CONFLICT	UNP Q9WUI9
K	739	ALA	LYS	CONFLICT	UNP Q9WUI9
L	739	ALA	LYS	CONFLICT	UNP Q9WUI9
M	739	ALA	LYS	CONFLICT	UNP Q9WUI9
N	739	ALA	LYS	CONFLICT	UNP Q9WUI9
O	739	ALA	LYS	CONFLICT	UNP Q9WUI9
P	739	ALA	LYS	CONFLICT	UNP Q9WUI9

- Molecule 4 is (9cis)-retinoic acid (three-letter code: 9CR) (formula: C₂₀H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			22	20	2		
4	B	1	Total	C	O	0	0
			22	20	2		
4	C	1	Total	C	O	0	0
			22	20	2		
4	D	1	Total	C	O	0	0
			22	20	2		

- Molecule 5 is 3,5-DICHLORO-2-{4-[(3,5-DICHLOROPYRIDIN-2-YL)OXY]PHENOXY}PYRIDINE (three-letter code: TCD) (formula: $C_{16}H_8Cl_4N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	Cl	N	O	0	0
			24	16	4	2	2		
5	F	1	Total	C	Cl	N	O	0	0
			24	16	4	2	2		
5	G	1	Total	C	Cl	N	O	0	0
			24	16	4	2	2		
5	H	1	Total	C	Cl	N	O	0	0
			24	16	4	2	2		

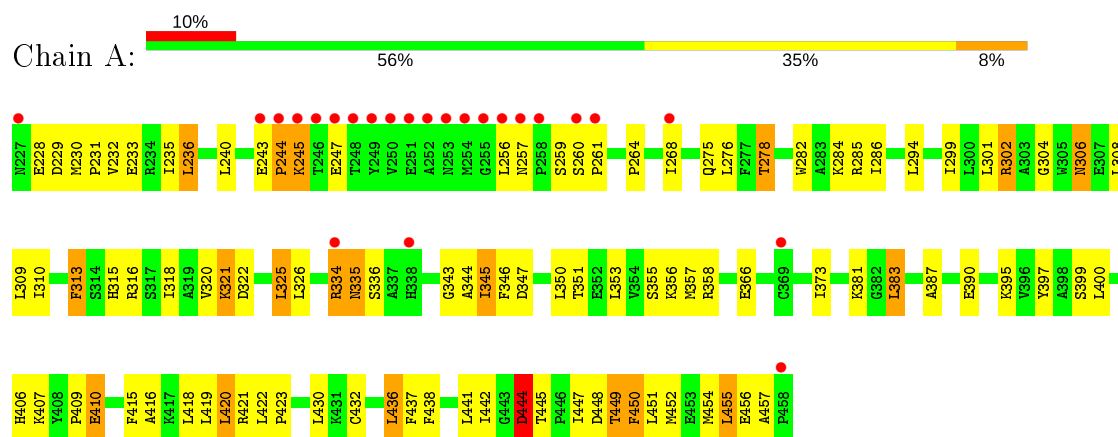
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	7	Total	O	0	0
			7	7		
6	B	8	Total	O	0	0
			8	8		
6	C	10	Total	O	0	0
			10	10		
6	D	20	Total	O	0	0
			20	20		
6	E	4	Total	O	0	0
			4	4		
6	F	17	Total	O	0	0
			17	17		
6	G	10	Total	O	0	0
			10	10		
6	H	4	Total	O	0	0
			4	4		
6	I	1	Total	O	0	0
			1	1		
6	J	1	Total	O	0	0
			1	1		
6	K	1	Total	O	0	0
			1	1		
6	L	1	Total	O	0	0
			1	1		
6	M	1	Total	O	0	0
			1	1		
6	O	1	Total	O	0	0
			1	1		
6	P	2	Total	O	0	0
			2	2		

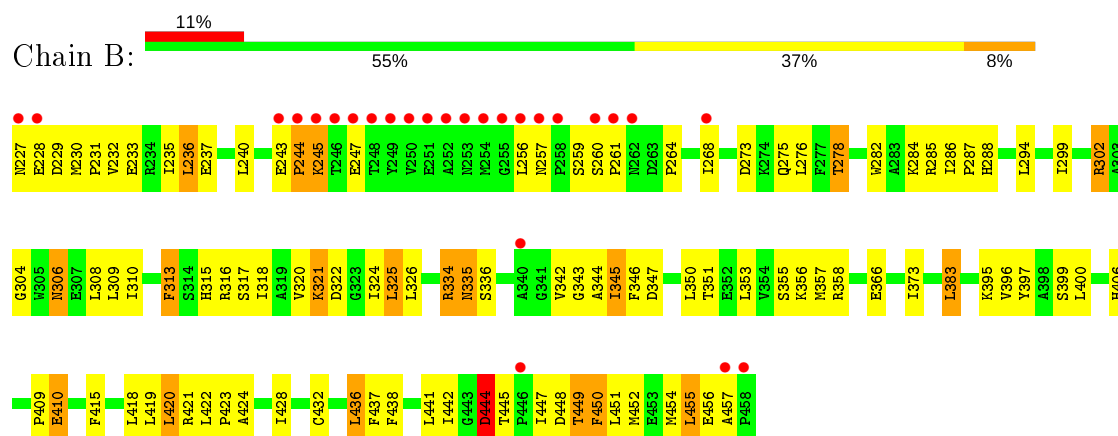
3 Residue-property plots

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

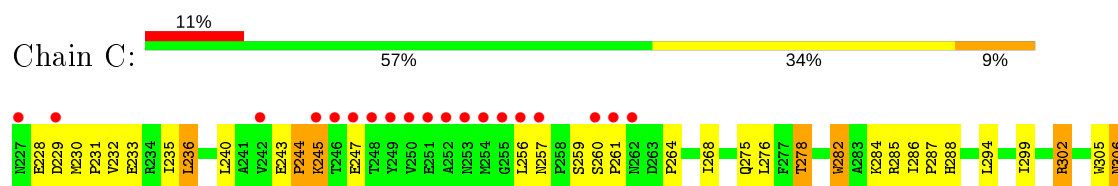
• Molecule 1: Retinoic acid receptor RXR-alpha

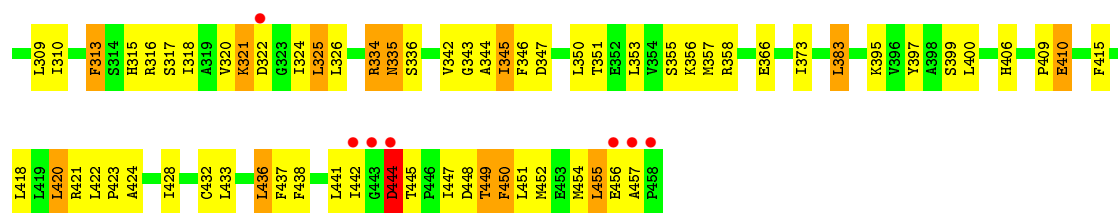


• Molecule 1: Retinoic acid receptor RXR-alpha

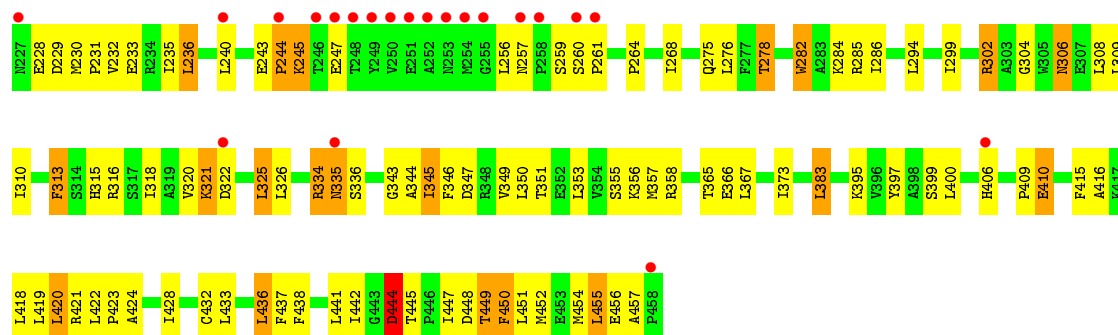


• Molecule 1: Retinoic acid receptor RXR-alpha

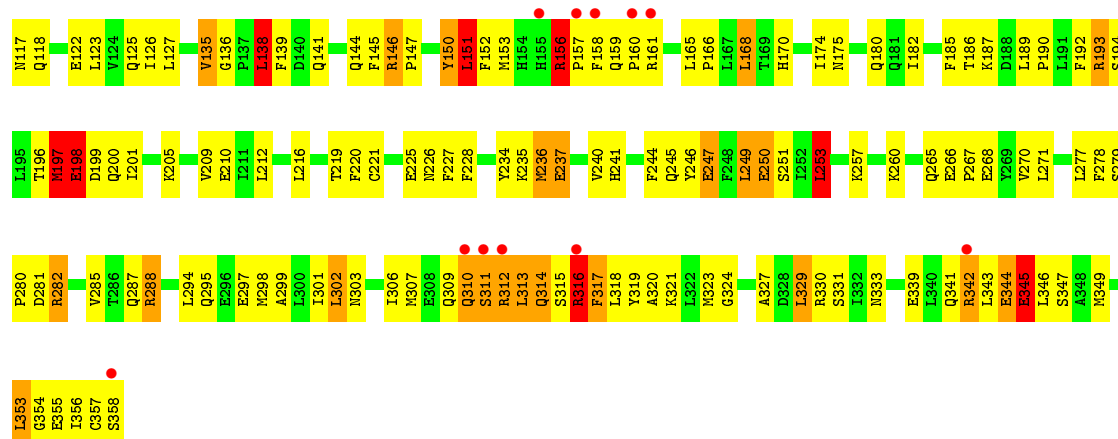
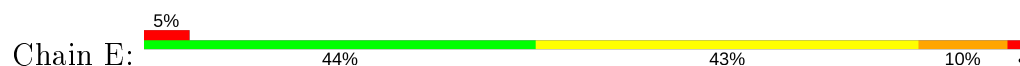




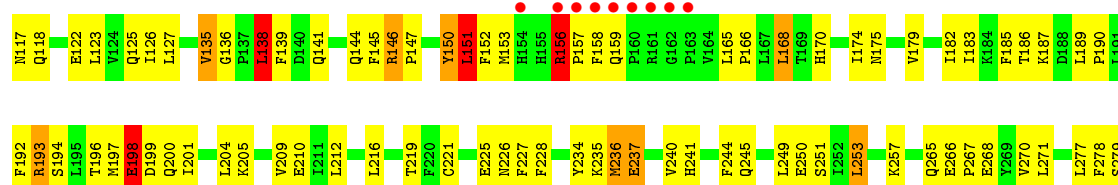
• Molecule 1: Retinoic acid receptor RXR-alpha

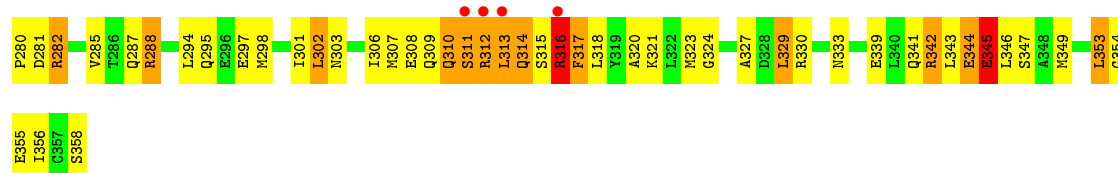


• Molecule 2: Orphan nuclear receptor NR1I3

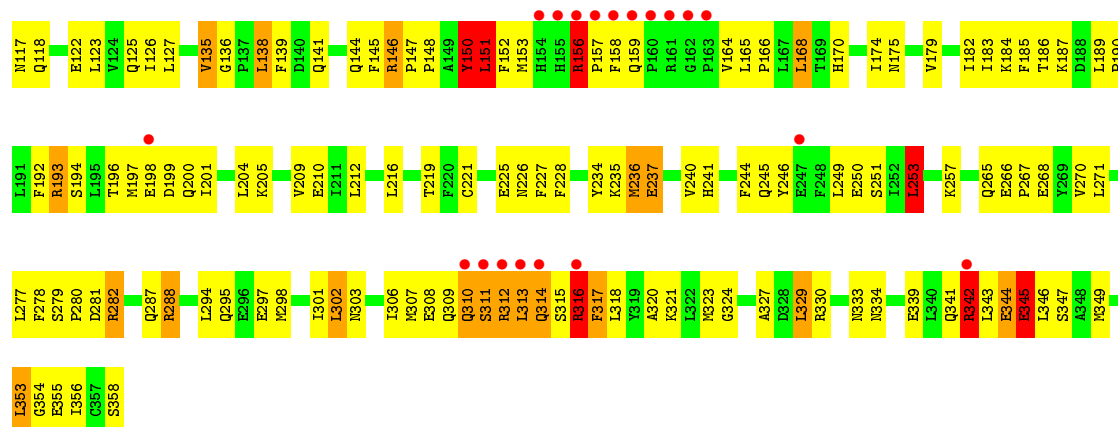


• Molecule 2: Orphan nuclear receptor NR1I3

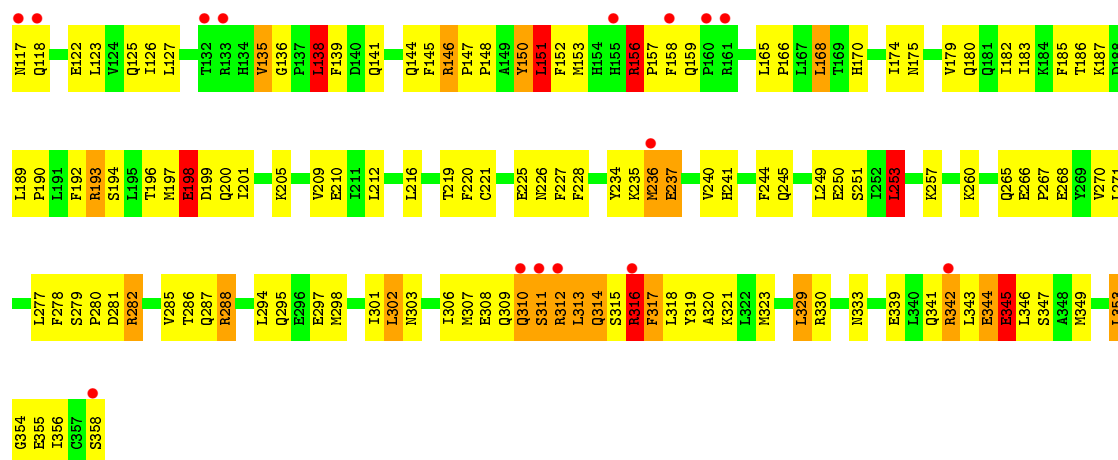
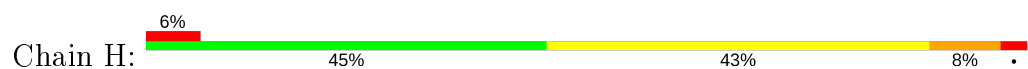




• Molecule 2: Orphan nuclear receptor NR1I3



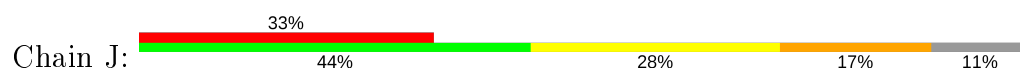
• Molecule 2: Orphan nuclear receptor NR1I3



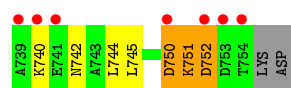
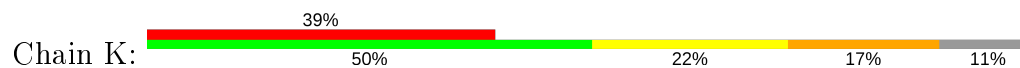
• Molecule 3: Nuclear receptor coactivator 2



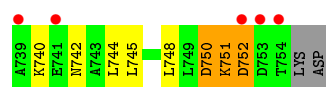
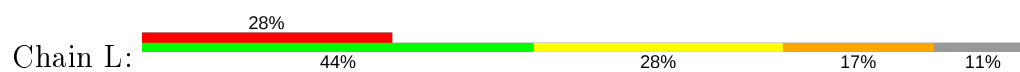
• Molecule 3: Nuclear receptor coactivator 2



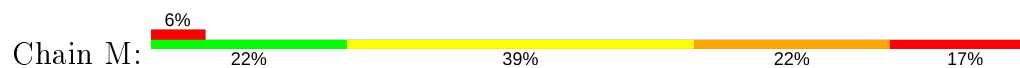
• Molecule 3: Nuclear receptor coactivator 2



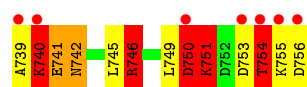
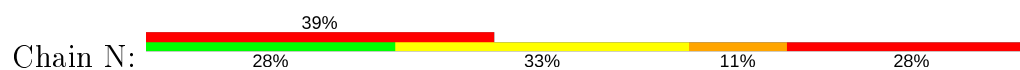
• Molecule 3: Nuclear receptor coactivator 2



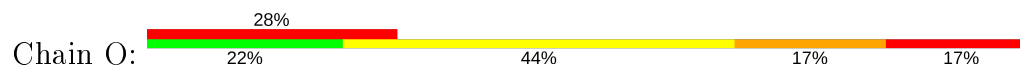
• Molecule 3: Nuclear receptor coactivator 2



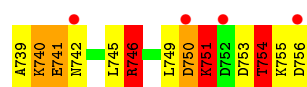
• Molecule 3: Nuclear receptor coactivator 2



• Molecule 3: Nuclear receptor coactivator 2



• Molecule 3: Nuclear receptor coactivator 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	68.27Å 88.38Å 105.49Å 79.02° 85.81° 67.22°	Depositor
Resolution (Å)	19.99 – 2.96 19.99 – 2.97	Depositor EDS
% Data completeness (in resolution range)	92.5 (19.99-2.96) 92.6 (19.99-2.97)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.303 0.250 , 0.293	Depositor DCC
R_{free} test set	3463 reflections (8.12%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	16288	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 9CR, TCD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/1790	0.60	0/2414
1	B	0.41	0/1790	0.61	0/2414
1	C	0.40	0/1790	0.60	0/2414
1	D	0.40	0/1790	0.61	0/2414
2	E	0.48	0/2016	0.94	16/2727 (0.6%)
2	F	0.48	1/2016 (0.0%)	0.85	8/2727 (0.3%)
2	G	0.48	2/2016 (0.1%)	0.83	6/2727 (0.2%)
2	H	0.54	1/2016 (0.0%)	1.28	14/2727 (0.5%)
3	I	0.39	0/131	0.60	0/175
3	J	0.40	0/131	0.62	0/175
3	K	0.34	0/131	0.61	0/175
3	L	0.39	0/131	0.60	0/175
3	M	1.01	1/149 (0.7%)	3.00	7/197 (3.6%)
3	N	0.84	1/149 (0.7%)	1.92	7/197 (3.6%)
3	O	0.84	1/149 (0.7%)	3.56	10/197 (5.1%)
3	P	0.99	1/149 (0.7%)	2.16	8/197 (4.1%)
All	All	0.48	8/16344 (0.0%)	0.96	76/22052 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1
3	M	0	1
3	N	0	1
3	P	0	1
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	193	ARG	CZ-NH1	-12.28	1.17	1.33
3	M	750	ASP	CB-CG	-7.52	1.35	1.51
3	P	750	ASP	CB-CG	-7.52	1.35	1.51
2	G	342	ARG	CB-CG	-6.12	1.36	1.52
3	N	750	ASP	CB-CG	-5.28	1.40	1.51
2	G	193	ARG	CZ-NH1	-5.24	1.26	1.33
3	O	750	ASP	CB-CG	-5.22	1.40	1.51
2	F	193	ARG	CZ-NH1	-5.07	1.26	1.33

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	193	ARG	NE-CZ-NH2	33.36	136.98	120.30
3	O	746	ARG	NE-CZ-NH1	-30.74	104.93	120.30
3	O	746	ARG	NE-CZ-NH2	27.55	134.08	120.30
3	M	746	ARG	NE-CZ-NH1	-26.46	107.07	120.30
2	H	342	ARG	NE-CZ-NH1	-24.98	107.81	120.30
3	M	746	ARG	NE-CZ-NH2	23.17	131.88	120.30
2	H	342	ARG	NE-CZ-NH2	20.96	130.78	120.30
3	O	750	ASP	CB-CG-OD1	-16.43	103.52	118.30
3	P	746	ARG	NE-CZ-NH1	-14.80	112.90	120.30
2	E	288	ARG	NE-CZ-NH1	14.32	127.46	120.30
2	F	288	ARG	NE-CZ-NH1	-14.06	113.27	120.30
2	H	288	ARG	NE-CZ-NH1	14.01	127.31	120.30
2	H	288	ARG	NE-CZ-NH2	-14.00	113.30	120.30
2	E	288	ARG	NE-CZ-NH2	-13.84	113.38	120.30
2	G	288	ARG	NE-CZ-NH1	-13.57	113.52	120.30
2	F	288	ARG	NE-CZ-NH2	13.57	127.08	120.30
3	M	750	ASP	CB-CG-OD1	-13.44	106.20	118.30
2	G	288	ARG	NE-CZ-NH2	13.29	126.95	120.30
3	P	750	ASP	CB-CG-OD1	-13.29	106.34	118.30
2	H	193	ARG	NE-CZ-NH1	-13.21	113.69	120.30
3	O	750	ASP	CB-CG-OD2	13.08	130.07	118.30
3	P	746	ARG	NE-CZ-NH2	12.33	126.47	120.30
3	N	746	ARG	NE-CZ-NH2	-11.67	114.47	120.30
3	N	750	ASP	CB-CG-OD1	-10.76	108.61	118.30
2	G	193	ARG	NE-CZ-NH2	10.68	125.64	120.30
2	F	193	ARG	NE-CZ-NH2	10.49	125.55	120.30
2	E	193	ARG	NE-CZ-NH2	10.44	125.52	120.30
2	H	342	ARG	CD-NE-CZ	9.76	137.26	123.60
2	E	197	MET	CG-SD-CE	-9.58	84.88	100.20
2	E	197	MET	CA-CB-CG	-9.53	97.09	113.30
2	H	253	LEU	CB-CG-CD2	-9.19	95.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	193	ARG	NH1-CZ-NH2	-9.17	109.31	119.40
2	F	198	GLU	CA-CB-CG	-8.28	95.19	113.40
3	N	746	ARG	NE-CZ-NH1	8.21	124.41	120.30
3	N	746	ARG	CD-NE-CZ	7.91	134.67	123.60
2	E	198	GLU	CG-CD-OE2	-7.69	102.92	118.30
2	H	288	ARG	CD-NE-CZ	7.57	134.19	123.60
2	E	288	ARG	CD-NE-CZ	7.51	134.12	123.60
2	E	247	GLU	CG-CD-OE2	-7.44	103.41	118.30
2	E	198	GLU	CG-CD-OE1	7.36	133.03	118.30
2	G	253	LEU	CB-CG-CD1	-7.17	98.81	111.00
2	H	198	GLU	CA-CB-CG	-7.13	97.71	113.40
2	F	288	ARG	CD-NE-CZ	7.05	133.46	123.60
3	M	750	ASP	CB-CG-OD2	7.01	124.61	118.30
3	N	746	ARG	CA-CB-CG	7.00	128.79	113.40
2	E	247	GLU	CG-CD-OE1	6.99	132.28	118.30
2	E	247	GLU	CB-CG-CD	-6.96	95.40	114.20
2	G	288	ARG	CD-NE-CZ	6.95	133.33	123.60
3	P	750	ASP	CB-CG-OD2	6.87	124.48	118.30
2	F	253	LEU	CB-CG-CD1	-6.69	99.63	111.00
3	M	746	ARG	CA-CB-CG	6.68	128.09	113.40
2	H	253	LEU	CB-CG-CD1	6.61	122.23	111.00
2	E	253	LEU	CB-CG-CD1	-6.60	99.79	111.00
2	E	198	GLU	CA-CB-CG	-6.53	99.05	113.40
3	P	746	ARG	CA-CB-CG	6.52	127.73	113.40
2	E	247	GLU	CA-CB-CG	6.44	127.56	113.40
2	G	342	ARG	CB-CG-CD	6.43	128.31	111.60
2	H	193	ARG	CG-CD-NE	6.21	124.83	111.80
3	M	746	ARG	CD-NE-CZ	6.19	132.27	123.60
3	N	750	ASP	CB-CG-OD2	6.19	123.87	118.30
3	O	746	ARG	CG-CD-NE	6.12	124.64	111.80
3	P	746	ARG	CD-NE-CZ	6.03	132.04	123.60
3	P	746	ARG	CB-CG-CD	-5.96	96.11	111.60
3	O	746	ARG	CB-CG-CD	-5.79	96.53	111.60
2	F	253	LEU	CB-CG-CD2	5.61	120.54	111.00
2	E	138	LEU	CA-CB-CG	5.61	128.19	115.30
3	P	754	THR	N-CA-C	-5.52	96.10	111.00
3	O	750	ASP	N-CA-C	5.48	125.79	111.00
2	E	197	MET	CB-CG-SD	5.42	128.67	112.40
3	M	754	THR	N-CA-C	-5.40	96.42	111.00
3	O	754	THR	N-CA-C	-5.34	96.57	111.00
2	H	138	LEU	CA-CB-CG	5.32	127.54	115.30
3	O	746	ARG	CA-CB-CG	5.27	124.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	754	THR	N-CA-C	-5.24	96.86	111.00
2	F	138	LEU	CA-CB-CG	5.20	127.26	115.30
3	O	750	ASP	CA-CB-CG	-5.05	102.29	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	150	TYR	Sidechain
3	M	746	ARG	Sidechain
3	N	746	ARG	Sidechain
3	P	746	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1755	0	1733	116	0
1	B	1755	0	1733	112	1
1	C	1755	0	1733	89	0
1	D	1755	0	1733	90	0
2	E	1969	0	1964	164	1
2	F	1969	0	1964	140	2
2	G	1969	0	1964	165	0
2	H	1969	0	1964	156	2
3	I	131	0	132	9	0
3	J	131	0	132	11	0
3	K	131	0	132	9	0
3	L	131	0	132	10	0
3	M	149	0	149	29	0
3	N	149	0	149	27	0
3	O	149	0	149	28	0
3	P	149	0	149	34	0
4	A	22	0	27	3	0
4	B	22	0	27	3	0
4	C	22	0	27	4	0
4	D	22	0	27	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	24	0	8	1	0
5	F	24	0	8	1	0
5	G	24	0	8	1	0
5	H	24	0	8	1	0
6	A	7	0	0	1	0
6	B	8	0	0	1	0
6	C	10	0	0	1	0
6	D	20	0	0	1	0
6	E	4	0	0	2	0
6	F	17	0	0	2	0
6	G	10	0	0	1	0
6	H	4	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	3	0
6	K	1	0	0	0	0
6	L	1	0	0	1	0
6	M	1	0	0	0	0
6	O	1	0	0	0	0
6	P	2	0	0	1	0
All	All	16288	0	16052	1058	3

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 33.

All (1058) 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)
2:E:157:PRO:CD	2:G:342:ARG:HH12	1.16	1.54
2:E:157:PRO:CD	2:G:342:ARG:NH1	1.74	1.39
2:E:157:PRO:HD3	2:G:342:ARG:NH1	1.09	1.37
1:A:406:HIS:CD2	1:B:233:GLU:HA	1.64	1.32
1:A:406:HIS:CE1	1:B:236:LEU:HB3	1.72	1.25
2:E:157:PRO:N	2:G:342:ARG:HH12	1.37	1.23
1:A:406:HIS:NE2	1:B:233:GLU:HA	1.60	1.17
2:E:342:ARG:HH22	2:G:157:PRO:HG3	1.12	1.11
2:H:253:LEU:O	2:H:253:LEU:HD23	1.50	1.08
2:H:253:LEU:O	2:H:253:LEU:CD2	2.11	0.99
2:E:157:PRO:HD3	2:G:342:ARG:HH11	1.16	0.95
2:H:187:LYS:HE2	3:P:749:LEU:O	1.68	0.94
1:A:406:HIS:CD2	1:B:233:GLU:CA	2.51	0.94
3:O:741:GLU:HG3	3:O:742:ASN:H	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:741:GLU:HG3	3:N:742:ASN:H	1.34	0.92
2:F:187:LYS:HE2	3:N:749:LEU:O	1.71	0.91
2:G:342:ARG:NH1	2:G:342:ARG:HG2	1.85	0.89
2:G:253:LEU:HD22	2:G:257:LYS:HE2	1.50	0.89
3:M:741:GLU:HG3	3:M:742:ASN:H	1.35	0.89
2:E:187:LYS:HE2	3:M:749:LEU:O	1.74	0.88
3:P:741:GLU:HG3	3:P:742:ASN:H	1.36	0.88
1:D:284:LYS:HZ2	3:L:752:ASP:HB2	1.39	0.88
1:C:284:LYS:NZ	3:K:752:ASP:HB2	1.88	0.88
1:B:284:LYS:NZ	3:J:752:ASP:HB2	1.89	0.88
2:H:253:LEU:CD2	2:H:253:LEU:C	2.41	0.86
1:A:406:HIS:CE1	1:B:233:GLU:O	2.28	0.85
2:G:187:LYS:HE2	3:O:749:LEU:O	1.76	0.85
2:E:342:ARG:HH22	2:G:157:PRO:CG	1.90	0.85
1:A:284:LYS:NZ	3:I:752:ASP:HB2	1.92	0.84
1:A:406:HIS:NE2	1:B:233:GLU:CA	2.40	0.83
1:D:284:LYS:NZ	3:L:752:ASP:HB2	1.93	0.83
1:C:438:PHE:O	1:C:442:ILE:HG13	1.79	0.82
1:A:406:HIS:CE1	1:B:236:LEU:CB	2.60	0.82
1:B:438:PHE:O	1:B:442:ILE:HG13	1.79	0.82
2:H:225:GLU:OE2	2:H:257:LYS:HD3	1.78	0.82
1:D:243:GLU:HB2	1:D:244:PRO:C	2.00	0.82
1:C:438:PHE:CD2	1:C:442:ILE:HD11	2.15	0.82
1:C:353:LEU:O	1:C:357:MET:HG3	1.81	0.81
1:A:406:HIS:ND1	1:B:233:GLU:O	2.13	0.81
1:A:438:PHE:CD2	1:A:442:ILE:HD11	2.16	0.81
2:G:244:PHE:HB2	2:G:249:LEU:HD21	1.63	0.81
2:G:253:LEU:O	2:G:253:LEU:HD23	1.82	0.80
1:B:438:PHE:CD2	1:B:442:ILE:HD11	2.16	0.80
1:A:243:GLU:HB2	1:A:244:PRO:C	2.01	0.80
1:D:438:PHE:O	1:D:442:ILE:HG13	1.81	0.80
1:C:243:GLU:HB2	1:C:244:PRO:C	2.02	0.80
1:A:438:PHE:O	1:A:442:ILE:HG13	1.82	0.80
2:F:244:PHE:HB2	2:F:249:LEU:HD21	1.63	0.80
1:B:353:LEU:O	1:B:357:MET:HG3	1.81	0.80
3:O:741:GLU:CG	3:O:742:ASN:H	1.94	0.80
1:B:243:GLU:HB2	1:B:244:PRO:C	2.02	0.79
2:F:225:GLU:OE2	2:F:257:LYS:HD3	1.82	0.79
2:H:253:LEU:HD23	2:H:253:LEU:C	1.93	0.79
1:A:233:GLU:HG3	1:B:227:ASN:N	1.98	0.79
2:G:311:SER:HA	2:G:314:GLN:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:741:GLU:CG	3:N:742:ASN:H	1.94	0.79
2:G:334:ASN:HB3	6:G:2:HOH:O	1.83	0.79
1:A:353:LEU:O	1:A:357:MET:HG3	1.83	0.79
1:A:299:ILE:HG21	1:A:383:LEU:HD13	1.64	0.79
1:D:438:PHE:CD2	1:D:442:ILE:HD11	2.19	0.78
2:E:311:SER:HA	2:E:314:GLN:HB3	1.64	0.78
2:E:225:GLU:OE2	2:E:257:LYS:HD3	1.83	0.78
2:G:342:ARG:HH11	2:G:342:ARG:CG	1.95	0.78
2:F:311:SER:HA	2:F:314:GLN:HB3	1.67	0.77
3:M:741:GLU:CG	3:M:742:ASN:H	1.96	0.77
2:H:311:SER:HA	2:H:314:GLN:HB3	1.66	0.77
1:A:437:PHE:O	1:A:441:LEU:HD23	1.84	0.77
2:E:244:PHE:HB2	2:E:249:LEU:HD21	1.65	0.77
1:D:299:ILE:HG21	1:D:383:LEU:HD13	1.65	0.76
2:G:225:GLU:OE2	2:G:257:LYS:HD3	1.85	0.76
3:P:741:GLU:CG	3:P:742:ASN:H	1.97	0.76
2:G:156:ARG:HB3	2:G:157:PRO:CA	2.16	0.76
2:G:342:ARG:HH11	2:G:342:ARG:HG2	1.45	0.76
2:H:253:LEU:HD21	2:H:257:LYS:HG3	1.67	0.76
3:N:750:ASP:O	3:N:751:LYS:C	2.24	0.76
1:C:299:ILE:HG21	1:C:383:LEU:HD13	1.66	0.76
2:F:156:ARG:HB3	2:F:157:PRO:CA	2.16	0.76
1:B:299:ILE:HG21	1:B:383:LEU:HD13	1.67	0.76
2:H:244:PHE:HB2	2:H:249:LEU:HD21	1.66	0.76
2:E:197:MET:SD	3:M:746:ARG:HG3	2.25	0.76
3:N:751:LYS:HE2	3:N:755:LYS:HZ3	1.52	0.75
2:H:156:ARG:HB3	2:H:157:PRO:CA	2.16	0.74
3:I:740:LYS:HE2	3:I:740:LYS:HA	1.67	0.74
3:O:750:ASP:O	3:O:751:LYS:C	2.26	0.74
1:C:422:LEU:HB2	1:C:423:PRO:HD3	1.70	0.74
1:D:449:THR:HG22	1:D:450:PHE:H	1.53	0.74
1:D:353:LEU:O	1:D:357:MET:HG3	1.87	0.74
2:E:156:ARG:HB3	2:E:157:PRO:CA	2.17	0.74
1:A:449:THR:HG22	1:A:450:PHE:H	1.53	0.74
2:E:182:ILE:O	2:E:185:PHE:HB3	1.87	0.74
3:J:740:LYS:HA	3:J:740:LYS:HE2	1.68	0.73
2:G:265:GLN:HG3	2:G:268:GLU:OE1	1.88	0.73
3:K:740:LYS:HE2	3:K:740:LYS:HA	1.69	0.73
1:D:437:PHE:O	1:D:441:LEU:HD23	1.88	0.73
1:D:243:GLU:HB2	1:D:245:LYS:N	2.04	0.73
1:A:243:GLU:HB2	1:A:245:LYS:N	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:PHE:O	1:B:441:LEU:HD23	1.88	0.73
3:L:740:LYS:HA	3:L:740:LYS:HE2	1.69	0.73
2:E:157:PRO:N	2:G:342:ARG:NH1	2.17	0.73
2:G:339:GLU:HB2	5:G:807:TCD:CL27	2.26	0.73
2:E:157:PRO:CG	2:G:342:ARG:HH12	1.99	0.72
1:A:335:ASN:ND2	1:A:336:SER:H	1.87	0.72
2:H:253:LEU:CD2	2:H:257:LYS:HG3	2.19	0.72
1:A:406:HIS:O	1:A:409:PRO:HD3	1.89	0.72
1:C:437:PHE:O	1:C:441:LEU:HD23	1.88	0.72
1:C:243:GLU:HB2	1:C:245:LYS:N	2.04	0.72
2:E:339:GLU:HB2	5:E:805:TCD:CL27	2.26	0.72
1:B:243:GLU:HB2	1:B:245:LYS:N	2.04	0.71
2:G:253:LEU:CD2	2:G:257:LYS:HG3	2.19	0.71
2:H:253:LEU:HD22	2:H:257:LYS:HE2	1.70	0.71
3:N:741:GLU:HG3	3:N:742:ASN:N	2.04	0.71
2:E:157:PRO:CG	2:G:342:ARG:NH1	2.51	0.71
2:E:156:ARG:C	2:G:342:ARG:HH22	1.94	0.71
2:F:197:MET:HE3	3:N:749:LEU:HD12	1.73	0.71
3:O:741:GLU:HG3	3:O:742:ASN:N	2.04	0.71
1:A:422:LEU:HB2	1:A:423:PRO:HD3	1.72	0.71
3:M:750:ASP:O	3:M:751:LYS:C	2.29	0.71
2:F:265:GLN:HG3	2:F:268:GLU:OE1	1.90	0.71
1:C:335:ASN:ND2	1:C:336:SER:H	1.89	0.71
1:B:335:ASN:ND2	1:B:336:SER:H	1.90	0.70
1:B:420:LEU:HA	2:F:323:MET:HE2	1.74	0.70
3:J:740:LYS:HE3	6:J:38:HOH:O	1.90	0.70
2:H:156:ARG:N	2:H:156:ARG:HD2	2.05	0.70
3:O:751:LYS:HE2	3:O:755:LYS:HZ3	1.57	0.70
2:F:156:ARG:N	2:F:156:ARG:HD2	2.06	0.70
1:D:335:ASN:ND2	1:D:336:SER:H	1.90	0.70
1:D:356:LYS:HG3	1:D:421:ARG:NH1	2.07	0.70
1:D:422:LEU:HB2	1:D:423:PRO:HD3	1.74	0.70
2:G:156:ARG:N	2:G:156:ARG:HD2	2.06	0.70
2:H:265:GLN:HG3	2:H:268:GLU:OE1	1.92	0.70
2:E:156:ARG:N	2:E:156:ARG:HD2	2.06	0.69
1:B:356:LYS:HG3	1:B:421:ARG:NH1	2.06	0.69
2:E:265:GLN:HG3	2:E:268:GLU:OE1	1.93	0.69
3:M:741:GLU:HG3	3:M:742:ASN:N	2.07	0.69
1:B:422:LEU:HB2	1:B:423:PRO:HD3	1.74	0.69
1:A:284:LYS:HZ2	3:I:752:ASP:HB2	1.58	0.69
3:P:741:GLU:HG3	3:P:742:ASN:N	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:THR:HG22	1:C:450:PHE:H	1.56	0.69
3:P:750:ASP:O	3:P:751:LYS:C	2.27	0.69
1:D:243:GLU:HB3	6:D:18:HOH:O	1.93	0.69
2:G:141:GLN:NE2	2:G:144:GLN:NE2	2.41	0.69
2:H:156:ARG:HB3	2:H:157:PRO:HA	1.75	0.69
2:E:156:ARG:HB3	2:E:157:PRO:HA	1.75	0.68
1:C:284:LYS:HZ3	3:K:752:ASP:HB2	1.57	0.68
1:B:284:LYS:HZ3	3:J:752:ASP:HB2	1.57	0.68
1:D:366:GLU:HG2	1:D:418:LEU:HD21	1.75	0.68
2:F:141:GLN:NE2	2:F:144:GLN:NE2	2.42	0.68
2:G:182:ILE:O	2:G:185:PHE:HB3	1.93	0.68
2:H:182:ILE:O	2:H:185:PHE:HB3	1.93	0.68
1:A:406:HIS:HE1	1:B:236:LEU:N	1.92	0.67
1:A:356:LYS:HG3	1:A:421:ARG:NH1	2.09	0.67
1:B:420:LEU:HA	2:F:323:MET:CE	2.24	0.67
1:D:406:HIS:O	1:D:409:PRO:HD3	1.93	0.67
2:H:253:LEU:HD22	2:H:253:LEU:C	2.14	0.67
2:H:158:PHE:CE2	2:H:241:HIS:NE2	2.62	0.67
2:H:197:MET:HE2	3:P:746:ARG:HG3	1.77	0.67
1:B:449:THR:HG22	1:B:450:PHE:H	1.57	0.67
2:G:141:GLN:NE2	2:G:144:GLN:HE21	1.93	0.67
2:H:141:GLN:NE2	2:H:144:GLN:NE2	2.43	0.67
1:C:264:PRO:O	1:C:268:ILE:HG13	1.94	0.67
2:E:197:MET:HE1	3:M:749:LEU:HB2	1.76	0.67
2:F:141:GLN:NE2	2:F:144:GLN:HE21	1.93	0.67
1:C:406:HIS:O	1:C:409:PRO:HD3	1.95	0.67
2:F:145:PHE:C	2:F:146:ARG:HD2	2.15	0.67
2:F:158:PHE:CE2	2:F:241:HIS:NE2	2.63	0.67
1:C:345:ILE:HD11	1:C:432:CYS:SG	2.35	0.66
1:C:450:PHE:O	1:C:454:MET:HG2	1.94	0.66
2:E:158:PHE:CE2	2:E:241:HIS:NE2	2.63	0.66
1:A:406:HIS:HE1	1:B:236:LEU:H	1.40	0.66
2:G:314:GLN:HG3	2:G:315:SER:H	1.60	0.66
2:E:145:PHE:C	2:E:146:ARG:HD2	2.16	0.66
1:D:450:PHE:O	1:D:454:MET:HG2	1.95	0.66
2:F:339:GLU:HB2	5:F:806:TCD:CL27	2.32	0.66
2:H:278:PHE:O	2:H:295:GLN:HB2	1.96	0.66
2:H:197:MET:HE3	3:P:749:LEU:HD12	1.78	0.66
1:C:351:THR:HA	1:C:355:SER:HB3	1.76	0.66
2:G:156:ARG:HB3	2:G:157:PRO:HA	1.76	0.66
2:H:339:GLU:HB2	5:H:808:TCD:CL27	2.32	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:ILE:HD13	1:C:345:ILE:O	1.96	0.66
2:E:141:GLN:NE2	2:E:144:GLN:NE2	2.44	0.66
1:A:420:LEU:HA	2:E:323:MET:CE	2.26	0.66
2:H:175:ASN:HD22	2:H:353:LEU:HD11	1.61	0.66
2:E:311:SER:O	2:E:312:ARG:HB2	1.96	0.65
1:B:282:TRP:CE2	1:B:286:ILE:HD11	2.30	0.65
1:A:335:ASN:HD22	1:A:336:SER:H	1.43	0.65
2:G:145:PHE:C	2:G:146:ARG:HD2	2.16	0.65
2:E:342:ARG:NH2	2:G:157:PRO:HG3	1.97	0.65
2:H:311:SER:O	2:H:312:ARG:HB2	1.96	0.65
3:P:751:LYS:HE2	3:P:755:LYS:HZ3	1.62	0.65
1:B:450:PHE:O	1:B:454:MET:HG2	1.96	0.65
2:H:237:GLU:O	2:H:240:VAL:HG22	1.94	0.65
2:E:278:PHE:O	2:E:295:GLN:HB2	1.97	0.65
1:A:420:LEU:HA	2:E:323:MET:HE2	1.78	0.65
1:B:264:PRO:O	1:B:268:ILE:HG13	1.96	0.65
2:F:156:ARG:HB3	2:F:157:PRO:HA	1.77	0.65
1:B:351:THR:HA	1:B:355:SER:HB3	1.78	0.65
1:B:447:ILE:HG13	1:B:447:ILE:O	1.96	0.65
2:F:314:GLN:HG3	2:F:315:SER:H	1.62	0.65
1:C:366:GLU:HG2	1:C:418:LEU:HD21	1.76	0.65
1:C:356:LYS:HG3	1:C:421:ARG:NH1	2.12	0.65
1:C:447:ILE:HD11	1:C:452:MET:SD	2.36	0.65
1:C:420:LEU:HA	2:G:323:MET:HE2	1.79	0.65
1:B:335:ASN:HD22	1:B:336:SER:H	1.44	0.64
1:C:447:ILE:O	1:C:447:ILE:HG13	1.96	0.64
2:H:314:GLN:HG3	2:H:315:SER:H	1.61	0.64
1:B:447:ILE:HD11	1:B:452:MET:SD	2.36	0.64
1:D:351:THR:HA	1:D:355:SER:HB3	1.78	0.64
1:C:335:ASN:HD22	1:C:336:SER:H	1.45	0.64
2:H:141:GLN:NE2	2:H:144:GLN:HE21	1.95	0.64
2:H:145:PHE:C	2:H:146:ARG:HD2	2.18	0.64
3:M:751:LYS:HE2	3:M:755:LYS:HZ3	1.63	0.64
2:E:314:GLN:HG3	2:E:315:SER:H	1.62	0.64
1:A:366:GLU:HG2	1:A:418:LEU:HD21	1.80	0.64
1:C:232:VAL:HG23	1:C:399:SER:HB3	1.80	0.64
1:A:351:THR:HA	1:A:355:SER:HB3	1.79	0.64
1:D:302:ARG:HB3	1:D:302:ARG:HH11	1.62	0.64
2:F:168:LEU:HD13	2:F:349:MET:CE	2.28	0.64
1:A:345:ILE:HD11	1:A:432:CYS:SG	2.38	0.64
1:D:264:PRO:O	1:D:268:ILE:HG13	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:VAL:CG2	1:C:399:SER:HB3	2.28	0.63
2:G:311:SER:O	2:G:312:ARG:HB2	1.96	0.63
1:B:406:HIS:O	1:B:409:PRO:HD3	1.98	0.63
2:G:158:PHE:CE2	2:G:241:HIS:NE2	2.66	0.63
1:B:232:VAL:HG23	1:B:399:SER:HB3	1.80	0.63
2:F:311:SER:O	2:F:312:ARG:HB2	1.97	0.63
2:G:278:PHE:O	2:G:295:GLN:HB2	1.98	0.63
1:B:366:GLU:HG2	1:B:418:LEU:HD21	1.78	0.63
1:C:436:LEU:HG	1:C:455:LEU:HD21	1.80	0.63
1:A:302:ARG:HH11	1:A:302:ARG:HB3	1.64	0.63
1:A:450:PHE:O	1:A:454:MET:HG2	1.98	0.63
1:D:335:ASN:N	1:D:335:ASN:HD22	1.95	0.63
3:L:752:ASP:HA	6:L:8:HOH:O	1.99	0.63
2:E:141:GLN:NE2	2:E:144:GLN:HE21	1.96	0.63
2:E:156:ARG:C	2:G:342:ARG:NH2	2.52	0.63
1:C:302:ARG:HH11	1:C:302:ARG:HB3	1.64	0.63
2:G:237:GLU:O	2:G:240:VAL:HG22	1.99	0.63
1:B:345:ILE:O	1:B:345:ILE:HD13	1.99	0.62
1:A:373:ILE:HD13	1:A:397:TYR:CE1	2.33	0.62
1:B:345:ILE:HD11	1:B:432:CYS:SG	2.38	0.62
1:D:232:VAL:CG2	1:D:399:SER:HB3	2.29	0.62
2:F:346:LEU:N	2:F:349:MET:HE2	2.15	0.62
2:G:168:LEU:HD13	2:G:349:MET:CE	2.30	0.62
2:E:246:TYR:HH	2:G:246:TYR:HE1	1.48	0.62
1:B:230:MET:CE	1:B:235:ILE:HD11	2.29	0.62
1:C:335:ASN:N	1:C:335:ASN:HD22	1.97	0.62
3:P:755:LYS:HZ3	3:P:755:LYS:HA	1.63	0.62
1:A:406:HIS:CG	1:B:233:GLU:O	2.52	0.62
2:G:151:LEU:HD12	2:G:156:ARG:HH22	1.64	0.62
2:H:168:LEU:HD13	2:H:349:MET:HE1	1.80	0.62
1:A:282:TRP:CE2	1:A:286:ILE:HD11	2.34	0.62
1:B:232:VAL:CG2	1:B:399:SER:HB3	2.30	0.62
1:A:232:VAL:CG2	1:A:399:SER:HB3	2.30	0.62
1:A:447:ILE:HD11	1:A:452:MET:SD	2.39	0.62
1:A:447:ILE:HG13	1:A:447:ILE:O	1.97	0.62
1:D:282:TRP:CE2	1:D:286:ILE:HD11	2.35	0.62
1:A:335:ASN:N	1:A:335:ASN:HD22	1.97	0.61
2:F:151:LEU:HD12	2:F:156:ARG:HH22	1.64	0.61
1:C:420:LEU:HA	2:G:323:MET:CE	2.30	0.61
1:D:335:ASN:HD22	1:D:336:SER:H	1.47	0.61
2:F:197:MET:CE	3:N:749:LEU:HD12	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:197:MET:HE3	3:O:749:LEU:HD12	1.83	0.61
2:F:278:PHE:O	2:F:295:GLN:HB2	1.99	0.61
1:A:264:PRO:O	1:A:268:ILE:HG13	2.00	0.61
1:C:373:ILE:HD13	1:C:397:TYR:CE1	2.35	0.61
2:E:237:GLU:O	2:E:240:VAL:HG22	1.99	0.61
3:M:755:LYS:HA	3:M:755:LYS:HZ3	1.64	0.61
1:B:335:ASN:N	1:B:335:ASN:HD22	1.98	0.61
2:E:187:LYS:HE2	3:M:749:LEU:HA	1.82	0.61
1:D:420:LEU:HA	2:H:323:MET:CE	2.30	0.61
2:E:316:ARG:HD3	2:E:317:PHE:N	2.16	0.61
2:F:314:GLN:C	2:F:316:ARG:N	2.53	0.61
2:G:314:GLN:C	2:G:316:ARG:N	2.52	0.61
1:D:230:MET:CE	1:D:235:ILE:HD11	2.30	0.61
1:B:436:LEU:HG	1:B:455:LEU:HD21	1.82	0.61
1:C:282:TRP:CE2	1:C:286:ILE:HD11	2.35	0.61
2:H:314:GLN:C	2:H:316:ARG:N	2.53	0.61
1:D:373:ILE:HD13	1:D:397:TYR:CE1	2.35	0.61
2:F:182:ILE:O	2:F:185:PHE:HB3	2.00	0.61
1:B:373:ILE:HD13	1:B:397:TYR:CE1	2.36	0.60
1:D:447:ILE:O	1:D:447:ILE:HG13	1.98	0.60
2:E:127:LEU:HB3	2:E:270:VAL:HG21	1.83	0.60
2:F:127:LEU:HB3	2:F:270:VAL:HG21	1.83	0.60
2:H:127:LEU:HD23	2:H:189:LEU:HD21	1.83	0.60
2:H:187:LYS:HE2	3:P:749:LEU:HA	1.83	0.60
1:B:302:ARG:HH11	1:B:302:ARG:HB3	1.67	0.60
1:D:447:ILE:HD11	1:D:452:MET:SD	2.40	0.60
2:E:357:CYS:HB2	6:E:83:HOH:O	2.01	0.60
1:A:406:HIS:CE1	1:B:233:GLU:C	2.75	0.60
1:B:284:LYS:HZ3	3:J:752:ASP:H	1.48	0.60
2:E:175:ASN:HD22	2:E:353:LEU:HD11	1.67	0.60
2:E:346:LEU:N	2:E:349:MET:HE2	2.15	0.60
1:A:406:HIS:NE2	1:B:232:VAL:O	2.34	0.60
2:G:127:LEU:HB3	2:G:270:VAL:HG21	1.84	0.60
1:B:306:ASN:H	1:B:306:ASN:HD22	1.50	0.60
2:H:151:LEU:HD12	2:H:156:ARG:HH22	1.66	0.60
1:D:345:ILE:HD11	1:D:432:CYS:SG	2.42	0.60
1:D:345:ILE:HD13	1:D:345:ILE:O	2.01	0.60
2:E:157:PRO:CB	2:G:342:ARG:HH12	2.15	0.60
1:A:438:PHE:CE2	1:A:442:ILE:HD11	2.37	0.60
2:F:117:ASN:OD1	2:F:118:GLN:N	2.34	0.60
2:G:193:ARG:HA	2:G:200:GLN:OE1	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ARG:HD2	1:B:325:LEU:O	2.02	0.59
2:E:151:LEU:HD12	2:E:156:ARG:HH22	1.66	0.59
2:E:311:SER:HB2	2:E:314:GLN:HE21	1.67	0.59
2:F:237:GLU:O	2:F:240:VAL:HG22	2.02	0.59
2:G:354:GLY:O	2:G:358:SER:HB2	2.02	0.59
2:H:190:PRO:O	2:H:194:SER:HB2	2.01	0.59
2:F:187:LYS:HE2	3:N:749:LEU:HA	1.83	0.59
3:P:755:LYS:NZ	3:P:755:LYS:HA	2.17	0.59
3:M:755:LYS:HA	3:M:755:LYS:NZ	2.17	0.59
1:A:233:GLU:CG	1:B:227:ASN:N	2.65	0.59
2:E:314:GLN:C	2:E:316:ARG:N	2.54	0.59
2:G:253:LEU:O	2:G:253:LEU:CD2	2.51	0.59
2:G:316:ARG:HD3	2:G:317:PHE:N	2.17	0.59
2:H:316:ARG:HD3	2:H:317:PHE:N	2.17	0.59
1:C:284:LYS:HZ3	3:K:752:ASP:H	1.49	0.59
2:H:127:LEU:HD23	2:H:189:LEU:CD2	2.33	0.59
3:L:750:ASP:O	3:L:751:LYS:HB3	2.03	0.59
3:J:750:ASP:O	3:J:751:LYS:HB3	2.03	0.59
2:H:150:TYR:HA	2:H:153:MET:CE	2.33	0.59
2:H:253:LEU:CD2	2:H:257:LYS:HE2	2.32	0.59
1:C:284:LYS:HZ2	3:K:752:ASP:HB2	1.66	0.59
3:L:744:LEU:HD23	3:L:744:LEU:C	2.23	0.59
2:F:354:GLY:O	2:F:358:SER:HB2	2.03	0.59
1:A:419:LEU:HD13	2:E:320:ALA:HA	1.85	0.59
1:A:436:LEU:HG	1:A:455:LEU:HD21	1.85	0.59
1:C:449:THR:O	1:C:451:LEU:N	2.34	0.59
2:F:190:PRO:O	2:F:194:SER:HB2	2.03	0.59
2:F:158:PHE:HE2	2:F:241:HIS:HE2	1.50	0.59
2:F:316:ARG:HD3	2:F:317:PHE:N	2.17	0.59
2:G:187:LYS:HE2	3:O:749:LEU:HA	1.84	0.58
1:A:321:LYS:NZ	6:A:44:HOH:O	2.26	0.58
2:E:190:PRO:O	2:E:194:SER:HB2	2.02	0.58
1:A:232:VAL:HG23	1:A:399:SER:HB3	1.84	0.58
2:F:297:GLU:O	2:F:301:ILE:HG13	2.02	0.58
2:H:346:LEU:N	2:H:349:MET:HE2	2.18	0.58
2:H:187:LYS:CE	3:P:749:LEU:O	2.47	0.58
2:E:127:LEU:HD23	2:E:189:LEU:CD2	2.34	0.58
1:C:230:MET:CE	1:C:235:ILE:HD11	2.34	0.58
2:G:297:GLU:O	2:G:301:ILE:HG13	2.02	0.58
2:H:236:MET:H	2:H:236:MET:CE	2.17	0.58
2:E:127:LEU:HD23	2:E:189:LEU:HD21	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:150:TYR:HA	2:E:153:MET:CE	2.33	0.58
2:G:190:PRO:O	2:G:194:SER:HB2	2.03	0.58
2:H:311:SER:HB2	2:H:314:GLN:HE21	1.68	0.58
1:D:436:LEU:HG	1:D:455:LEU:HD21	1.86	0.58
2:E:354:GLY:O	2:E:358:SER:HB2	2.03	0.58
2:H:314:GLN:O	2:H:315:SER:OG	2.21	0.58
1:D:232:VAL:HG23	1:D:399:SER:HB3	1.85	0.58
1:D:275:GLN:HA	1:D:278:THR:HG23	1.86	0.58
2:F:175:ASN:HD22	2:F:353:LEU:HD11	1.68	0.58
2:F:197:MET:HE2	3:N:746:ARG:HG3	1.84	0.58
1:D:316:ARG:HD2	1:D:325:LEU:O	2.03	0.58
2:G:117:ASN:OD1	2:G:118:GLN:N	2.37	0.58
2:G:314:GLN:C	2:G:316:ARG:H	2.06	0.58
2:G:346:LEU:N	2:G:349:MET:HE2	2.19	0.58
3:M:754:THR:HG23	3:M:756:ASP:O	2.04	0.58
2:H:127:LEU:HB3	2:H:270:VAL:HG21	1.86	0.58
2:H:187:LYS:HE2	3:P:749:LEU:C	2.25	0.58
1:A:230:MET:CE	1:A:235:ILE:HD11	2.33	0.57
1:A:335:ASN:ND2	1:A:336:SER:N	2.51	0.57
2:E:117:ASN:OD1	2:E:118:GLN:N	2.36	0.57
2:H:354:GLY:O	2:H:358:SER:HB2	2.04	0.57
3:I:750:ASP:O	3:I:751:LYS:HB3	2.04	0.57
3:K:750:ASP:O	3:K:751:LYS:HB3	2.05	0.57
1:A:345:ILE:HD13	1:A:345:ILE:O	2.04	0.57
2:E:297:GLU:O	2:E:301:ILE:HG13	2.03	0.57
2:G:175:ASN:HD22	2:G:353:LEU:HD11	1.69	0.57
1:D:438:PHE:CE2	1:D:442:ILE:HD11	2.40	0.57
2:H:117:ASN:OD1	2:H:118:GLN:N	2.37	0.57
1:D:302:ARG:HB3	1:D:302:ARG:NH1	2.20	0.57
1:D:236:LEU:HD22	1:D:240:LEU:HD13	1.87	0.57
2:H:158:PHE:HE2	2:H:241:HIS:HE2	1.49	0.57
2:H:345:GLU:HB2	2:H:349:MET:CE	2.35	0.57
1:A:302:ARG:HB3	1:A:302:ARG:NH1	2.20	0.57
2:G:197:MET:CE	3:O:749:LEU:HD12	2.34	0.57
1:A:236:LEU:HD22	1:A:236:LEU:O	2.04	0.57
1:D:306:ASN:H	1:D:306:ASN:HD22	1.52	0.57
1:C:421:ARG:HA	1:C:421:ARG:NE	2.20	0.57
1:C:438:PHE:CE2	1:C:442:ILE:HD11	2.40	0.57
2:F:314:GLN:C	2:F:316:ARG:H	2.06	0.57
2:H:314:GLN:C	2:H:316:ARG:H	2.07	0.57
3:N:755:LYS:NZ	3:N:755:LYS:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:345:GLU:HB2	2:E:349:MET:CE	2.35	0.56
2:F:150:TYR:HA	2:F:153:MET:CE	2.36	0.56
2:H:197:MET:CE	3:P:749:LEU:HD12	2.34	0.56
3:P:754:THR:HG23	3:P:756:ASP:O	2.05	0.56
2:G:125:GLN:HE21	2:G:126:ILE:CD1	2.19	0.56
1:B:421:ARG:HA	1:B:421:ARG:NE	2.21	0.56
2:E:236:MET:CE	2:E:236:MET:H	2.19	0.56
2:E:310:GLN:O	2:E:311:SER:O	2.23	0.56
1:D:420:LEU:HA	2:H:323:MET:HE2	1.86	0.56
2:F:197:MET:HE3	3:N:749:LEU:CD1	2.35	0.56
2:E:125:GLN:HE21	2:E:126:ILE:CD1	2.19	0.56
2:E:193:ARG:HA	2:E:200:GLN:OE1	2.05	0.56
2:H:168:LEU:HD13	2:H:349:MET:CE	2.35	0.56
1:B:284:LYS:HZ2	3:J:752:ASP:HB2	1.69	0.56
1:A:236:LEU:HD22	1:A:240:LEU:HD13	1.88	0.56
2:E:314:GLN:C	2:E:316:ARG:H	2.08	0.56
2:G:150:TYR:HA	2:G:153:MET:CE	2.36	0.56
2:G:310:GLN:O	2:G:311:SER:O	2.24	0.56
1:A:275:GLN:HA	1:A:278:THR:HG23	1.88	0.56
1:A:316:ARG:HD2	1:A:325:LEU:O	2.05	0.56
1:C:302:ARG:HB3	1:C:302:ARG:NH1	2.21	0.56
2:E:345:GLU:HB2	2:E:349:MET:HE1	1.87	0.56
3:P:746:ARG:CG	3:P:746:ARG:HH11	2.19	0.56
2:F:193:ARG:HA	2:F:200:GLN:OE1	2.05	0.56
2:F:196:THR:HG22	2:F:198:GLU:HG3	1.87	0.56
1:C:316:ARG:HD2	1:C:325:LEU:O	2.06	0.55
2:E:314:GLN:O	2:E:315:SER:OG	2.23	0.55
1:B:302:ARG:HA	1:B:454:MET:HE1	1.89	0.55
1:C:229:ASP:HB3	1:C:395:LYS:HD3	1.87	0.55
2:E:170:HIS:O	2:E:174:ILE:HG12	2.07	0.55
2:E:168:LEU:HD13	2:E:349:MET:CE	2.35	0.55
2:F:158:PHE:HE2	2:F:241:HIS:NE2	2.04	0.55
2:E:246:TYR:CG	2:G:237:GLU:HG3	2.41	0.55
1:B:449:THR:O	1:B:451:LEU:N	2.36	0.55
2:G:158:PHE:HE2	2:G:241:HIS:HE2	1.54	0.55
2:H:125:GLN:HE21	2:H:126:ILE:CD1	2.20	0.55
1:C:320:VAL:HG22	1:C:321:LYS:N	2.21	0.55
2:H:297:GLU:O	2:H:301:ILE:HG13	2.06	0.55
1:B:444:ASP:O	6:B:1:HOH:O	2.18	0.55
2:F:266:GLU:O	2:F:270:VAL:HG12	2.06	0.55
1:B:397:TYR:HB3	2:F:317:PHE:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:345:GLU:HB2	2:F:349:MET:CE	2.37	0.55
2:H:158:PHE:HE2	2:H:241:HIS:NE2	2.04	0.55
1:B:438:PHE:CE2	1:B:442:ILE:HD11	2.41	0.55
1:D:302:ARG:HA	1:D:454:MET:HE1	1.87	0.55
1:B:335:ASN:ND2	1:B:336:SER:N	2.54	0.55
2:G:311:SER:HB2	2:G:314:GLN:HE21	1.70	0.55
1:B:236:LEU:HD22	1:B:236:LEU:O	2.06	0.55
3:O:755:LYS:HA	3:O:755:LYS:NZ	2.21	0.55
1:A:320:VAL:HG22	1:A:321:LYS:N	2.22	0.55
1:C:335:ASN:ND2	1:C:336:SER:N	2.54	0.55
1:D:335:ASN:ND2	1:D:336:SER:N	2.54	0.55
2:F:315:SER:HB2	2:F:321:LYS:NZ	2.21	0.55
2:F:280:PRO:HB3	2:F:288:ARG:HG2	1.89	0.54
2:E:156:ARG:CA	2:G:342:ARG:HH22	2.20	0.54
2:H:271:LEU:HD13	2:H:302:LEU:HA	1.89	0.54
2:E:271:LEU:HD13	2:E:302:LEU:HA	1.89	0.54
2:F:168:LEU:HD13	2:F:349:MET:HE1	1.88	0.54
2:F:187:LYS:HE2	3:N:749:LEU:C	2.27	0.54
2:G:236:MET:CE	2:G:236:MET:H	2.20	0.54
2:G:168:LEU:HD13	2:G:349:MET:HE1	1.89	0.54
2:H:310:GLN:O	2:H:311:SER:O	2.25	0.54
2:E:236:MET:HG2	2:E:253:LEU:HD13	1.87	0.54
3:O:754:THR:HG23	3:O:756:ASP:O	2.06	0.54
3:P:746:ARG:HG2	3:P:746:ARG:HH11	1.72	0.54
2:H:197:MET:HE3	3:P:749:LEU:CD1	2.37	0.54
2:E:127:LEU:HB3	2:E:270:VAL:CG2	2.38	0.54
1:A:306:ASN:H	1:A:306:ASN:HD22	1.55	0.54
1:B:320:VAL:HG22	1:B:321:LYS:N	2.22	0.54
1:C:236:LEU:HD22	1:C:236:LEU:O	2.07	0.54
1:C:236:LEU:HD22	1:C:240:LEU:HD13	1.88	0.54
2:F:356:ILE:HD11	3:N:745:LEU:HD21	1.89	0.54
1:B:229:ASP:HB3	1:B:395:LYS:HD3	1.89	0.54
2:E:158:PHE:HE2	2:E:241:HIS:HE2	1.51	0.54
1:D:397:TYR:HB3	2:H:317:PHE:CD1	2.42	0.54
3:N:754:THR:HG23	3:N:756:ASP:O	2.06	0.54
2:E:187:LYS:HE2	3:M:749:LEU:C	2.28	0.54
2:F:236:MET:H	2:F:236:MET:CE	2.21	0.54
2:F:311:SER:HB2	2:F:314:GLN:HE21	1.72	0.54
3:O:755:LYS:HA	3:O:755:LYS:HZ3	1.73	0.54
1:D:229:ASP:HB3	1:D:395:LYS:HD3	1.89	0.54
3:J:744:LEU:C	3:J:744:LEU:HD23	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ASN:HD22	1:C:306:ASN:H	1.56	0.54
2:E:158:PHE:HE2	2:E:241:HIS:NE2	2.05	0.54
2:E:245:GLN:O	2:E:249:LEU:CD2	2.55	0.54
2:F:310:GLN:O	2:F:311:SER:O	2.26	0.54
2:G:317:PHE:HB3	2:G:320:ALA:HB3	1.90	0.54
2:G:345:GLU:HB2	2:G:349:MET:CE	2.38	0.54
3:K:744:LEU:HD23	3:K:744:LEU:C	2.28	0.54
1:A:302:ARG:HA	1:A:454:MET:HE1	1.88	0.54
1:D:421:ARG:HA	1:D:421:ARG:NE	2.22	0.54
2:F:201:ILE:HG22	2:F:205:LYS:HD2	1.89	0.54
1:A:284:LYS:HZ3	3:I:752:ASP:H	1.54	0.53
1:A:421:ARG:HA	1:A:421:ARG:NE	2.23	0.53
2:E:157:PRO:CB	2:G:342:ARG:NH1	2.70	0.53
2:F:127:LEU:HD23	2:F:189:LEU:CD2	2.38	0.53
2:G:147:PRO:HB3	2:G:170:HIS:CE1	2.43	0.53
2:F:125:GLN:HE21	2:F:126:ILE:CD1	2.22	0.53
1:A:449:THR:O	1:A:451:LEU:N	2.35	0.53
2:G:356:ILE:HD11	3:O:745:LEU:HD21	1.90	0.53
2:G:127:LEU:HD23	2:G:189:LEU:CD2	2.38	0.53
2:E:187:LYS:CE	3:M:749:LEU:O	2.52	0.53
2:E:302:LEU:O	2:E:306:ILE:HG13	2.09	0.53
2:G:156:ARG:CB	2:G:157:PRO:HA	2.39	0.53
1:D:304:GLY:O	1:D:308:LEU:HG	2.08	0.53
2:G:201:ILE:HG22	2:G:205:LYS:HD2	1.90	0.53
2:G:271:LEU:HD13	2:G:302:LEU:HA	1.91	0.53
2:G:315:SER:HB2	2:G:321:LYS:NZ	2.23	0.53
3:N:750:ASP:O	3:N:751:LYS:O	2.26	0.53
1:B:275:GLN:HA	1:B:278:THR:HG23	1.90	0.53
1:A:381:LYS:NZ	2:E:247:GLU:OE1	2.33	0.53
2:F:156:ARG:HB3	2:F:157:PRO:C	2.29	0.53
2:G:156:ARG:HB3	2:G:157:PRO:C	2.29	0.53
3:P:746:ARG:NH1	3:P:746:ARG:CG	2.71	0.53
2:E:306:ILE:HD13	2:E:318:LEU:HD12	1.90	0.53
2:H:197:MET:HE1	3:P:749:LEU:HB2	1.90	0.53
2:H:302:LEU:O	2:H:306:ILE:HG13	2.09	0.53
2:H:201:ILE:HG22	2:H:205:LYS:HD2	1.91	0.53
1:D:320:VAL:HG22	1:D:321:LYS:N	2.24	0.53
2:F:127:LEU:HB3	2:F:270:VAL:CG2	2.39	0.53
1:C:275:GLN:HA	1:C:278:THR:HG23	1.90	0.52
2:G:280:PRO:HB3	2:G:288:ARG:HG2	1.91	0.52
2:H:168:LEU:HD22	2:H:346:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:240:VAL:CG2	2:H:241:HIS:N	2.72	0.52
1:A:284:LYS:HZ3	3:I:752:ASP:HB2	1.72	0.52
2:F:302:LEU:O	2:F:306:ILE:HG13	2.09	0.52
2:H:156:ARG:CB	2:H:157:PRO:HA	2.39	0.52
2:H:306:ILE:HD13	2:H:318:LEU:HD12	1.91	0.52
1:A:229:ASP:HB3	1:A:395:LYS:HD3	1.90	0.52
1:C:285:ARG:NH1	6:C:13:HOH:O	2.43	0.52
1:D:326:LEU:HD22	4:D:804:9CR:H25	1.92	0.52
2:E:156:ARG:CB	2:E:157:PRO:HA	2.39	0.52
2:F:156:ARG:CB	2:F:157:PRO:HA	2.39	0.52
2:F:306:ILE:HD13	2:F:318:LEU:HD12	1.91	0.52
2:F:168:LEU:HD13	2:F:349:MET:HE3	1.92	0.52
2:H:158:PHE:CG	2:H:159:GLN:N	2.77	0.52
1:D:419:LEU:HD13	2:H:320:ALA:HA	1.91	0.52
2:E:150:TYR:HA	2:E:153:MET:HE3	1.91	0.52
2:F:127:LEU:HD23	2:F:189:LEU:HD21	1.90	0.52
1:B:236:LEU:HD22	1:B:240:LEU:HD13	1.91	0.52
2:H:127:LEU:HB3	2:H:270:VAL:CG2	2.40	0.52
1:B:302:ARG:HB3	1:B:302:ARG:NH1	2.24	0.52
2:F:245:GLN:O	2:F:249:LEU:CD2	2.57	0.52
2:G:210:GLU:HG2	2:G:329:LEU:HB3	1.92	0.52
2:H:345:GLU:C	2:H:349:MET:HE2	2.30	0.52
2:G:158:PHE:HE2	2:G:241:HIS:NE2	2.07	0.52
1:B:409:PRO:HD2	1:B:410:GLU:OE2	2.10	0.52
2:F:210:GLU:HG2	2:F:329:LEU:HB3	1.92	0.52
2:G:127:LEU:HD23	2:G:189:LEU:HD21	1.91	0.52
2:G:245:GLN:O	2:G:249:LEU:CD2	2.58	0.52
3:O:750:ASP:O	3:O:751:LYS:O	2.28	0.52
1:A:326:LEU:HD22	4:A:801:9CR:H25	1.92	0.52
1:C:309:LEU:HD23	4:C:803:9CR:H11	1.92	0.52
2:F:345:GLU:HB2	2:F:349:MET:HE1	1.91	0.52
2:H:266:GLU:O	2:H:270:VAL:HG12	2.09	0.52
3:I:744:LEU:C	3:I:744:LEU:HD23	2.30	0.52
1:C:315:HIS:O	1:C:318:ILE:HG13	2.09	0.51
2:E:311:SER:HB2	2:E:314:GLN:NE2	2.25	0.51
2:E:168:LEU:HD22	2:E:346:LEU:HD13	1.91	0.51
1:B:309:LEU:HD23	4:B:802:9CR:H11	1.93	0.51
2:E:158:PHE:CG	2:E:159:GLN:N	2.78	0.51
2:E:201:ILE:HG22	2:E:205:LYS:HD2	1.92	0.51
2:F:314:GLN:O	2:F:315:SER:OG	2.23	0.51
2:G:314:GLN:O	2:G:315:SER:OG	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:315:SER:O	2:H:317:PHE:N	2.43	0.51
2:H:193:ARG:NH2	3:P:750:ASP:OD1	2.36	0.51
2:G:306:ILE:HD13	2:G:318:LEU:HD12	1.92	0.51
2:H:193:ARG:HA	2:H:200:GLN:OE1	2.10	0.51
1:D:315:HIS:O	1:D:318:ILE:HG13	2.11	0.51
2:E:316:ARG:O	2:E:318:LEU:N	2.37	0.51
2:H:147:PRO:HB3	2:H:170:HIS:CE1	2.45	0.51
2:E:165:LEU:HB3	2:E:166:PRO:HD3	1.92	0.51
2:F:271:LEU:HD13	2:F:302:LEU:HA	1.93	0.51
2:F:317:PHE:HB3	2:F:320:ALA:HB3	1.93	0.51
2:G:187:LYS:HE2	3:O:749:LEU:C	2.31	0.51
2:F:187:LYS:CE	3:N:749:LEU:O	2.50	0.51
1:B:326:LEU:HD22	4:B:802:9CR:H25	1.92	0.51
3:P:750:ASP:O	3:P:751:LYS:O	2.28	0.51
1:A:304:GLY:O	1:A:308:LEU:HG	2.10	0.51
2:G:302:LEU:O	2:G:306:ILE:HG13	2.10	0.51
2:F:187:LYS:HE2	3:N:749:LEU:CA	2.40	0.51
2:G:266:GLU:O	2:G:270:VAL:HG12	2.10	0.51
2:E:157:PRO:CA	2:G:342:ARG:HH12	2.17	0.51
2:G:168:LEU:HD13	2:G:349:MET:HE3	1.93	0.51
2:H:135:VAL:O	2:H:138:LEU:HG	2.11	0.51
2:H:311:SER:HB2	2:H:314:GLN:NE2	2.26	0.51
2:F:150:TYR:HA	2:F:153:MET:HE2	1.93	0.51
2:G:127:LEU:HB3	2:G:270:VAL:CG2	2.41	0.50
2:H:170:HIS:O	2:H:174:ILE:HG12	2.11	0.50
1:C:302:ARG:HA	1:C:454:MET:HE1	1.93	0.50
2:E:317:PHE:HB3	2:E:320:ALA:HB3	1.94	0.50
2:F:147:PRO:HB3	2:F:170:HIS:CE1	2.46	0.50
2:F:315:SER:O	2:F:317:PHE:N	2.45	0.50
2:H:150:TYR:HA	2:H:153:MET:HE3	1.93	0.50
1:C:346:PHE:HE1	1:C:350:LEU:HD11	1.76	0.50
2:E:266:GLU:O	2:E:270:VAL:HG12	2.10	0.50
2:E:316:ARG:C	2:E:316:ARG:HD3	2.32	0.50
2:H:253:LEU:O	2:H:253:LEU:HD22	2.03	0.50
2:H:317:PHE:HB3	2:H:320:ALA:HB3	1.94	0.50
1:C:444:ASP:O	1:C:445:THR:C	2.49	0.50
2:G:165:LEU:HB3	2:G:166:PRO:HD3	1.94	0.50
2:H:165:LEU:HB3	2:H:166:PRO:HD3	1.92	0.50
2:H:313:LEU:HD23	2:H:314:GLN:H	1.77	0.50
1:A:416:ALA:HB1	2:E:319:TYR:CZ	2.46	0.50
2:H:253:LEU:HD21	2:H:257:LYS:CG	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:313:LEU:HD12	6:F:67:HOH:O	2.10	0.50
2:G:158:PHE:CG	2:G:159:GLN:N	2.79	0.50
2:H:187:LYS:HE2	3:P:749:LEU:CA	2.41	0.50
1:A:315:HIS:O	1:A:318:ILE:HG13	2.12	0.50
1:A:335:ASN:HD22	1:A:336:SER:N	2.10	0.50
2:E:315:SER:O	2:E:317:PHE:N	2.44	0.50
2:F:158:PHE:CG	2:F:159:GLN:N	2.80	0.50
1:D:449:THR:O	1:D:451:LEU:N	2.38	0.50
1:C:326:LEU:HD22	4:C:803:9CR:H25	1.93	0.50
2:E:135:VAL:O	2:E:138:LEU:HG	2.12	0.50
2:E:313:LEU:HD23	2:E:314:GLN:H	1.77	0.50
2:G:199:ASP:OD1	2:G:287:GLN:HG2	2.11	0.50
2:H:156:ARG:CB	2:H:157:PRO:CA	2.90	0.50
2:H:245:GLN:O	2:H:249:LEU:CD2	2.59	0.50
1:C:284:LYS:CD	3:K:752:ASP:HB2	2.42	0.49
2:E:315:SER:HB2	2:E:321:LYS:NZ	2.27	0.49
2:F:165:LEU:HB3	2:F:166:PRO:HD3	1.94	0.49
2:G:316:ARG:O	2:G:318:LEU:N	2.36	0.49
2:H:226:ASN:ND2	2:H:235:LYS:HG2	2.26	0.49
2:E:227:PHE:HB2	2:E:234:TYR:HB2	1.94	0.49
2:G:253:LEU:HD23	2:G:257:LYS:HG3	1.93	0.49
2:G:168:LEU:HD22	2:G:346:LEU:HD13	1.94	0.49
1:A:313:PHE:C	1:A:313:PHE:CD1	2.86	0.49
2:F:315:SER:HB2	2:F:321:LYS:HZ2	1.77	0.49
2:H:316:ARG:C	2:H:316:ARG:HD3	2.33	0.49
1:B:318:ILE:HG23	1:B:358:ARG:HB2	1.94	0.49
2:F:225:GLU:HB3	2:F:253:LEU:HD11	1.95	0.49
2:F:271:LEU:HB3	2:F:302:LEU:HD23	1.94	0.49
2:G:187:LYS:HE2	3:O:749:LEU:CA	2.42	0.49
2:H:345:GLU:HB2	2:H:349:MET:HE2	1.93	0.49
3:M:750:ASP:O	3:M:751:LYS:O	2.30	0.49
1:B:231:PRO:C	1:B:233:GLU:N	2.63	0.49
2:G:170:HIS:O	2:G:174:ILE:HG12	2.12	0.49
1:A:406:HIS:HE1	1:B:236:LEU:CB	2.18	0.49
1:B:315:HIS:O	1:B:318:ILE:HG13	2.12	0.49
1:B:444:ASP:O	1:B:445:THR:C	2.50	0.49
2:F:313:LEU:CD1	6:F:67:HOH:O	2.60	0.49
2:G:240:VAL:CG2	2:G:241:HIS:N	2.76	0.49
2:H:186:THR:HB	2:H:192:PHE:CD2	2.48	0.49
3:M:741:GLU:CG	3:M:742:ASN:N	2.65	0.49
2:E:186:THR:HB	2:E:192:PHE:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:196:THR:HG22	2:G:198:GLU:HG2	1.93	0.49
2:H:307:MET:C	2:H:309:GLN:H	2.16	0.49
3:N:755:LYS:HA	3:N:755:LYS:HZ3	1.77	0.49
1:D:313:PHE:C	1:D:313:PHE:CD1	2.86	0.49
2:E:156:ARG:HB3	2:E:157:PRO:C	2.32	0.49
1:A:309:LEU:HD23	4:A:801:9CR:H11	1.95	0.49
2:E:240:VAL:CG2	2:E:241:HIS:N	2.76	0.49
2:G:324:GLY:O	2:G:327:ALA:HB3	2.12	0.49
2:H:316:ARG:O	2:H:318:LEU:N	2.39	0.49
2:F:324:GLY:O	2:F:327:ALA:HB3	2.13	0.48
3:P:741:GLU:CG	3:P:742:ASN:N	2.65	0.48
1:A:373:ILE:HD13	1:A:397:TYR:HE1	1.78	0.48
1:D:306:ASN:N	1:D:306:ASN:HD22	2.12	0.48
2:H:156:ARG:HB3	2:H:157:PRO:C	2.32	0.48
2:H:356:ILE:HD11	3:P:745:LEU:HD21	1.94	0.48
1:A:299:ILE:HG21	1:A:383:LEU:CD1	2.39	0.48
2:G:315:SER:O	2:G:317:PHE:N	2.47	0.48
2:H:279:SER:HB2	2:H:282:ARG:HD2	1.94	0.48
1:B:284:LYS:CD	3:J:752:ASP:HB2	2.43	0.48
1:C:313:PHE:CD1	1:C:313:PHE:C	2.86	0.48
2:E:122:GLU:O	2:E:126:ILE:HD13	2.13	0.48
2:F:226:ASN:ND2	2:F:235:LYS:HG2	2.29	0.48
2:F:307:MET:C	2:F:309:GLN:H	2.16	0.48
2:H:227:PHE:HB2	2:H:234:TYR:HB2	1.95	0.48
1:C:231:PRO:C	1:C:233:GLU:N	2.67	0.48
1:C:318:ILE:HG23	1:C:358:ARG:HB2	1.95	0.48
1:D:299:ILE:HG21	1:D:383:LEU:CD1	2.39	0.48
2:G:196:THR:HB	2:G:199:ASP:HB2	1.95	0.48
2:H:210:GLU:HG2	2:H:329:LEU:HB3	1.95	0.48
1:D:284:LYS:HZ3	3:L:752:ASP:H	1.60	0.48
2:F:313:LEU:HD23	2:F:314:GLN:H	1.78	0.48
2:F:316:ARG:O	2:F:318:LEU:N	2.37	0.48
2:G:315:SER:HB2	2:G:321:LYS:HZ2	1.79	0.48
1:C:409:PRO:HD2	1:C:410:GLU:OE2	2.13	0.48
2:G:135:VAL:O	2:G:138:LEU:HG	2.13	0.48
2:H:150:TYR:HA	2:H:153:MET:HE2	1.96	0.48
1:D:309:LEU:HD23	4:D:804:9CR:H11	1.96	0.48
2:F:240:VAL:CG2	2:F:241:HIS:N	2.77	0.48
2:G:186:THR:HB	2:G:192:PHE:CD2	2.49	0.48
2:E:245:GLN:O	2:E:249:LEU:HD22	2.14	0.48
1:A:397:TYR:HB3	2:E:317:PHE:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:311:SER:HB2	2:F:314:GLN:NE2	2.29	0.48
2:H:122:GLU:O	2:H:126:ILE:HD13	2.14	0.48
1:A:334:ARG:HG2	1:A:334:ARG:HH11	1.78	0.48
1:D:444:ASP:O	1:D:445:THR:C	2.50	0.48
2:E:299:ALA:HB3	6:E:50:HOH:O	2.14	0.48
2:E:168:LEU:HD13	2:E:349:MET:HE1	1.96	0.48
2:G:197:MET:HE3	3:O:749:LEU:CD1	2.43	0.48
2:G:329:LEU:HD12	2:G:329:LEU:HA	1.77	0.48
1:A:284:LYS:CD	3:I:752:ASP:HB2	2.43	0.47
2:E:187:LYS:HE2	3:M:749:LEU:CA	2.42	0.47
2:F:199:ASP:OD1	2:F:287:GLN:HG2	2.14	0.47
2:G:219:THR:HB	2:G:228:PHE:O	2.14	0.47
2:G:311:SER:HB2	2:G:314:GLN:NE2	2.29	0.47
2:G:345:GLU:HB2	2:G:349:MET:HE1	1.95	0.47
3:J:740:LYS:HG2	6:J:38:HOH:O	2.13	0.47
1:A:444:ASP:O	1:A:445:THR:C	2.51	0.47
1:D:236:LEU:O	1:D:236:LEU:HD22	2.14	0.47
2:E:307:MET:C	2:E:309:GLN:H	2.17	0.47
2:H:315:SER:HB2	2:H:321:LYS:NZ	2.29	0.47
2:E:160:PRO:HB2	2:G:164:VAL:HG11	1.95	0.47
2:F:168:LEU:HD22	2:F:346:LEU:HD13	1.96	0.47
3:M:740:LYS:HB2	3:M:740:LYS:HZ3	1.80	0.47
1:D:334:ARG:HH11	1:D:334:ARG:HG2	1.78	0.47
2:E:147:PRO:HB3	2:E:170:HIS:CE1	2.49	0.47
2:E:139:PHE:CE2	2:E:216:LEU:HA	2.50	0.47
2:F:345:GLU:C	2:F:349:MET:HE2	2.35	0.47
2:G:122:GLU:O	2:G:126:ILE:HD13	2.14	0.47
2:G:139:PHE:CE2	2:G:216:LEU:HA	2.49	0.47
2:G:244:PHE:CB	2:G:249:LEU:HD21	2.40	0.47
2:E:279:SER:HB2	2:E:282:ARG:HD2	1.95	0.47
1:D:284:LYS:CD	3:L:752:ASP:HB2	2.44	0.47
3:P:740:LYS:HZ3	3:P:740:LYS:HB2	1.80	0.47
1:B:424:ALA:O	1:B:428:ILE:HG13	2.15	0.47
2:E:210:GLU:HG2	2:E:329:LEU:HB3	1.97	0.47
2:E:245:GLN:O	2:E:249:LEU:HD23	2.15	0.47
2:F:244:PHE:CB	2:F:249:LEU:HD21	2.41	0.47
2:G:150:TYR:O	2:G:152:PHE:N	2.48	0.47
2:G:245:GLN:O	2:G:249:LEU:HD23	2.14	0.47
2:F:356:ILE:CD1	3:N:745:LEU:HD21	2.45	0.47
1:B:419:LEU:HD13	2:F:320:ALA:HA	1.97	0.47
2:E:135:VAL:O	2:E:136:GLY:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:196:THR:HB	2:E:199:ASP:HB2	1.96	0.47
2:F:139:PHE:CE2	2:F:216:LEU:HA	2.50	0.47
2:F:186:THR:HB	2:F:192:PHE:CD2	2.50	0.47
2:G:156:ARG:CB	2:G:157:PRO:CA	2.89	0.47
1:A:343:GLY:O	1:A:344:ALA:HB3	2.15	0.47
1:B:373:ILE:HD13	1:B:397:TYR:HE1	1.78	0.47
2:E:168:LEU:HD13	2:E:349:MET:HE3	1.97	0.47
2:F:135:VAL:O	2:F:138:LEU:HG	2.14	0.47
2:E:282:ARG:O	2:E:285:VAL:HG13	2.15	0.47
2:E:356:ILE:HD11	3:M:745:LEU:HD21	1.96	0.47
1:A:306:ASN:HD22	1:A:306:ASN:N	2.13	0.47
1:C:424:ALA:O	1:C:428:ILE:HG13	2.15	0.47
2:E:265:GLN:NE2	2:E:309:GLN:OE1	2.43	0.47
2:G:265:GLN:NE2	2:G:309:GLN:OE1	2.47	0.47
3:N:741:GLU:CG	3:N:742:ASN:N	2.62	0.47
2:G:187:LYS:CE	3:O:749:LEU:O	2.54	0.47
1:A:228:GLU:O	1:A:228:GLU:HG2	2.15	0.47
1:B:313:PHE:CD1	1:B:313:PHE:C	2.88	0.47
1:D:373:ILE:HD13	1:D:397:TYR:HE1	1.80	0.47
2:F:245:GLN:O	2:F:249:LEU:HD23	2.14	0.47
2:G:307:MET:C	2:G:309:GLN:H	2.17	0.46
2:H:341:GLN:C	2:H:343:LEU:H	2.19	0.46
3:P:753:ASP:C	3:P:754:THR:HG22	2.35	0.46
1:B:326:LEU:HD22	4:B:802:9CR:C20	2.44	0.46
1:C:326:LEU:HD22	4:C:803:9CR:C20	2.44	0.46
2:F:329:LEU:HA	2:F:329:LEU:HD12	1.79	0.46
2:G:226:ASN:ND2	2:G:235:LYS:HG2	2.30	0.46
3:L:744:LEU:O	3:L:744:LEU:HD23	2.14	0.46
1:A:406:HIS:HE1	1:B:236:LEU:CA	2.29	0.46
1:C:335:ASN:ND2	1:C:335:ASN:N	2.63	0.46
2:F:156:ARG:CB	2:F:157:PRO:CA	2.89	0.46
2:G:135:VAL:O	2:G:136:GLY:C	2.51	0.46
2:G:345:GLU:C	2:G:349:MET:HE2	2.36	0.46
2:H:346:LEU:O	2:H:347:SER:C	2.54	0.46
1:B:343:GLY:O	1:B:344:ALA:HB3	2.15	0.46
1:C:343:GLY:O	1:C:344:ALA:HB3	2.15	0.46
1:D:409:PRO:HD2	1:D:410:GLU:OE2	2.16	0.46
2:E:345:GLU:C	2:E:349:MET:HE2	2.34	0.46
2:F:122:GLU:O	2:F:126:ILE:HD13	2.14	0.46
2:G:150:TYR:HA	2:G:153:MET:HE2	1.97	0.46
3:P:740:LYS:N	3:P:740:LYS:HD3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:271:LEU:HB3	2:H:302:LEU:HD23	1.96	0.46
1:B:228:GLU:HG2	1:B:228:GLU:O	2.16	0.46
2:F:135:VAL:O	2:F:136:GLY:C	2.52	0.46
2:H:212:LEU:HD23	2:H:212:LEU:C	2.36	0.46
1:A:302:ARG:HA	1:A:454:MET:CE	2.45	0.46
1:C:334:ARG:HG2	1:C:334:ARG:HH11	1.80	0.46
1:C:373:ILE:HD13	1:C:397:TYR:HE1	1.78	0.46
2:E:316:ARG:HH11	2:E:317:PHE:HD1	1.64	0.46
2:E:281:ASP:N	2:E:281:ASP:OD1	2.49	0.46
2:E:341:GLN:C	2:E:343:LEU:H	2.20	0.46
2:F:219:THR:HB	2:F:228:PHE:O	2.16	0.46
2:F:209:VAL:HB	2:F:333:ASN:ND2	2.31	0.46
1:A:318:ILE:HG23	1:A:358:ARG:HB2	1.98	0.46
1:D:326:LEU:HD22	4:D:804:9CR:C20	2.45	0.46
2:F:221:CYS:O	2:F:225:GLU:N	2.48	0.46
2:G:279:SER:HB2	2:G:282:ARG:HD2	1.98	0.46
2:G:271:LEU:HB3	2:G:302:LEU:HD23	1.98	0.46
2:G:356:ILE:CD1	3:O:745:LEU:HD21	2.46	0.46
2:F:316:ARG:HD3	2:F:316:ARG:C	2.35	0.46
3:O:741:GLU:CG	3:O:742:ASN:N	2.62	0.46
1:A:326:LEU:HD22	4:A:801:9CR:C20	2.46	0.45
1:A:406:HIS:CE1	1:B:236:LEU:H	2.28	0.45
1:D:335:ASN:HD22	1:D:336:SER:N	2.14	0.45
1:D:343:GLY:O	1:D:344:ALA:HB3	2.16	0.45
2:E:316:ARG:C	2:E:318:LEU:H	2.19	0.45
2:F:265:GLN:NE2	2:F:309:GLN:OE1	2.48	0.45
2:G:221:CYS:O	2:G:225:GLU:N	2.48	0.45
2:G:316:ARG:C	2:G:318:LEU:H	2.18	0.45
3:N:751:LYS:CE	3:N:755:LYS:HZ3	2.27	0.45
3:P:739:ALA:O	3:P:741:GLU:N	2.44	0.45
2:H:196:THR:HG22	2:H:198:GLU:HG3	1.99	0.45
2:F:346:LEU:O	2:F:347:SER:C	2.53	0.45
3:M:739:ALA:O	3:M:741:GLU:N	2.45	0.45
1:B:304:GLY:O	1:B:308:LEU:HG	2.15	0.45
1:B:334:ARG:HH11	1:B:334:ARG:HG2	1.81	0.45
1:B:345:ILE:C	1:B:345:ILE:HD13	2.37	0.45
1:D:231:PRO:C	1:D:233:GLU:N	2.69	0.45
2:F:196:THR:HB	2:F:199:ASP:HB2	1.98	0.45
2:F:265:GLN:HB2	2:F:267:PRO:HD2	1.99	0.45
2:G:150:TYR:HA	2:G:153:MET:HE3	1.98	0.45
1:B:231:PRO:C	1:B:233:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ASN:N	1:D:335:ASN:ND2	2.62	0.45
2:E:346:LEU:O	2:E:347:SER:C	2.55	0.45
2:F:312:ARG:O	2:F:313:LEU:HB3	2.17	0.45
2:F:341:GLN:C	2:F:343:LEU:H	2.19	0.45
2:H:139:PHE:CE2	2:H:216:LEU:HA	2.52	0.45
2:H:346:LEU:HA	2:H:349:MET:CE	2.46	0.45
1:A:231:PRO:C	1:A:233:GLU:N	2.69	0.45
1:A:406:HIS:ND1	1:B:237:GLU:HG2	2.31	0.45
1:B:335:ASN:N	1:B:335:ASN:ND2	2.64	0.45
1:C:345:ILE:HD13	1:C:345:ILE:C	2.37	0.45
1:C:433:LEU:HA	1:C:433:LEU:HD23	1.87	0.45
2:E:156:ARG:CB	2:E:157:PRO:CA	2.91	0.45
2:G:253:LEU:CD2	2:G:257:LYS:HE2	2.36	0.45
2:G:312:ARG:O	2:G:313:LEU:HB3	2.17	0.45
2:G:313:LEU:HD23	2:G:314:GLN:H	1.81	0.45
2:G:316:ARG:HD3	2:G:316:ARG:C	2.36	0.45
2:H:316:ARG:C	2:H:318:LEU:H	2.20	0.45
1:D:346:PHE:HE1	1:D:350:LEU:HD11	1.82	0.45
2:E:219:THR:HB	2:E:228:PHE:O	2.16	0.45
2:F:316:ARG:C	2:F:318:LEU:H	2.19	0.45
2:G:196:THR:CG2	2:G:198:GLU:HG2	2.47	0.45
2:F:227:PHE:HB2	2:F:234:TYR:HB2	1.98	0.45
2:G:212:LEU:HD23	2:G:212:LEU:C	2.36	0.45
2:H:294:LEU:O	2:H:298:MET:HB2	2.17	0.45
3:J:739:ALA:N	6:J:38:HOH:O	2.48	0.45
2:E:199:ASP:OD1	2:E:287:GLN:HG2	2.17	0.45
2:G:197:MET:HE1	3:O:749:LEU:HB2	1.99	0.45
2:H:312:ARG:O	2:H:313:LEU:HB3	2.17	0.45
1:D:228:GLU:HG2	1:D:228:GLU:O	2.17	0.45
1:D:302:ARG:HA	1:D:454:MET:CE	2.46	0.45
2:F:279:SER:HB2	2:F:282:ARG:HD2	1.99	0.45
2:H:346:LEU:HA	2:H:349:MET:HE3	1.99	0.45
3:M:753:ASP:C	3:M:754:THR:HG22	2.37	0.45
1:B:346:PHE:HE1	1:B:350:LEU:HD11	1.82	0.44
1:C:317:SER:OG	1:C:324:ILE:HA	2.17	0.44
2:E:150:TYR:HA	2:E:153:MET:HE2	1.99	0.44
2:H:240:VAL:HG23	2:H:241:HIS:N	2.32	0.44
2:H:245:GLN:O	2:H:249:LEU:HD22	2.17	0.44
3:M:746:ARG:HH11	3:M:746:ARG:CG	2.30	0.44
3:N:739:ALA:O	3:N:741:GLU:N	2.45	0.44
1:C:302:ARG:HA	1:C:454:MET:CE	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:803:9CR:H8	4:C:803:9CR:H10	1.82	0.44
1:D:345:ILE:HD13	1:D:345:ILE:C	2.38	0.44
2:E:279:SER:HA	2:E:280:PRO:HD3	1.84	0.44
2:G:253:LEU:C	2:G:253:LEU:CD2	2.86	0.44
2:H:196:THR:HB	2:H:199:ASP:HB2	1.98	0.44
2:H:221:CYS:O	2:H:225:GLU:N	2.49	0.44
2:H:280:PRO:HB3	2:H:288:ARG:HG2	1.99	0.44
2:E:212:LEU:HD23	2:E:212:LEU:C	2.38	0.44
2:G:279:SER:HA	2:G:280:PRO:HD3	1.83	0.44
2:G:346:LEU:O	2:G:347:SER:C	2.55	0.44
2:H:309:GLN:HE21	2:H:309:GLN:HB2	1.59	0.44
3:M:746:ARG:HG2	3:M:746:ARG:HH11	1.81	0.44
1:B:335:ASN:HD22	1:B:336:SER:N	2.12	0.44
1:C:228:GLU:HG2	1:C:228:GLU:O	2.17	0.44
2:E:271:LEU:HB3	2:E:302:LEU:HD23	1.99	0.44
2:E:346:LEU:HA	2:E:349:MET:CE	2.47	0.44
2:G:253:LEU:C	2:G:253:LEU:HD23	2.38	0.44
2:G:209:VAL:HB	2:G:333:ASN:ND2	2.32	0.44
1:B:302:ARG:HA	1:B:454:MET:CE	2.46	0.44
1:D:400:LEU:HD23	1:D:415:PHE:HE1	1.82	0.44
2:F:294:LEU:O	2:F:298:MET:HB2	2.18	0.44
2:G:227:PHE:HB2	2:G:234:TYR:HB2	1.99	0.44
2:H:265:GLN:NE2	2:H:309:GLN:OE1	2.46	0.44
3:N:753:ASP:C	3:N:754:THR:HG22	2.38	0.44
1:A:346:PHE:HE1	1:A:350:LEU:HD11	1.82	0.44
1:D:449:THR:HG22	1:D:450:PHE:N	2.27	0.44
2:F:318:LEU:O	2:F:318:LEU:HD13	2.18	0.44
1:C:397:TYR:HB3	2:G:317:PHE:CD1	2.52	0.44
2:F:346:LEU:HA	2:F:349:MET:CE	2.48	0.44
2:H:279:SER:HA	2:H:280:PRO:HD3	1.84	0.44
3:O:739:ALA:O	3:O:741:GLU:N	2.44	0.44
2:F:204:LEU:HD12	2:F:204:LEU:HA	1.81	0.44
2:G:294:LEU:O	2:G:298:MET:HB2	2.18	0.44
2:H:201:ILE:HG23	3:P:745:LEU:HD13	1.99	0.44
1:D:424:ALA:O	1:D:428:ILE:HG13	2.18	0.44
2:E:309:GLN:HE21	2:E:309:GLN:HB2	1.59	0.44
2:H:317:PHE:O	2:H:321:LYS:HG3	2.18	0.44
3:O:753:ASP:C	3:O:754:THR:HG22	2.39	0.44
1:A:285:ARG:HH11	1:A:285:ARG:HG2	1.83	0.43
1:A:335:ASN:N	1:A:335:ASN:ND2	2.63	0.43
1:A:345:ILE:HD13	1:A:345:ILE:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:318:LEU:C	2:F:318:LEU:HD13	2.38	0.43
2:G:281:ASP:N	2:G:281:ASP:OD1	2.50	0.43
2:H:135:VAL:O	2:H:136:GLY:C	2.55	0.43
2:H:353:LEU:HD23	2:H:353:LEU:HA	1.85	0.43
3:P:740:LYS:HD2	6:P:34:HOH:O	2.18	0.43
1:B:230:MET:HE2	1:B:396:VAL:HG22	1.99	0.43
1:B:447:ILE:CG1	1:B:447:ILE:O	2.66	0.43
2:E:244:PHE:CB	2:E:249:LEU:HD21	2.43	0.43
1:B:415:PHE:HE2	2:F:316:ARG:HH12	1.66	0.43
1:D:276:LEU:HA	1:D:276:LEU:HD12	1.87	0.43
1:B:436:LEU:HA	1:B:436:LEU:HD12	1.90	0.43
1:C:447:ILE:O	1:C:447:ILE:CG1	2.66	0.43
2:E:180:GLN:HE21	2:E:180:GLN:HB3	1.65	0.43
2:E:226:ASN:ND2	2:E:235:LYS:HG2	2.33	0.43
2:H:265:GLN:HB2	2:H:267:PRO:HD2	2.00	0.43
2:H:281:ASP:N	2:H:281:ASP:OD1	2.52	0.43
3:M:740:LYS:N	3:M:740:LYS:HD3	2.34	0.43
2:H:199:ASP:OD1	2:H:287:GLN:HG2	2.18	0.43
2:H:345:GLU:HB2	2:H:349:MET:HE1	1.99	0.43
1:C:320:VAL:CG2	1:C:321:LYS:N	2.81	0.43
1:D:318:ILE:HG23	1:D:358:ARG:HB2	2.00	0.43
2:H:150:TYR:O	2:H:152:PHE:N	2.51	0.43
2:H:244:PHE:CB	2:H:249:LEU:HD21	2.44	0.43
2:H:316:ARG:HH11	2:H:317:PHE:HD1	1.67	0.43
1:A:449:THR:HG22	1:A:450:PHE:N	2.28	0.43
1:C:285:ARG:HH11	1:C:285:ARG:HG2	1.84	0.43
1:A:400:LEU:HD23	1:A:415:PHE:HE1	1.83	0.43
1:C:346:PHE:CE1	1:C:350:LEU:HD11	2.52	0.43
1:C:366:GLU:CG	1:C:418:LEU:HD21	2.47	0.43
2:H:245:GLN:O	2:H:249:LEU:HD23	2.19	0.43
2:H:282:ARG:O	2:H:285:VAL:HG13	2.19	0.43
3:N:740:LYS:N	3:N:740:LYS:HD3	2.32	0.43
3:O:740:LYS:HD3	3:O:740:LYS:N	2.32	0.43
3:O:746:ARG:HH11	3:O:746:ARG:HD2	1.42	0.43
1:A:320:VAL:CG2	1:A:321:LYS:N	2.81	0.43
1:B:287:PRO:O	1:B:288:HIS:HB2	2.18	0.43
2:F:192:PHE:C	2:F:194:SER:H	2.22	0.43
2:G:265:GLN:HB2	2:G:267:PRO:HD2	2.01	0.43
1:A:299:ILE:CG2	1:A:383:LEU:HD13	2.44	0.43
1:B:285:ARG:HG2	1:B:285:ARG:HH11	1.83	0.43
2:G:341:GLN:C	2:G:343:LEU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:148:PRO:HD2	2:H:151:LEU:HD22	2.01	0.43
2:H:209:VAL:HB	2:H:333:ASN:ND2	2.34	0.43
1:B:321:LYS:HG3	1:B:322:ASP:N	2.34	0.42
2:E:198:GLU:HG3	2:E:198:GLU:H	1.01	0.42
2:E:265:GLN:HB2	2:E:267:PRO:HD2	2.00	0.42
2:F:150:TYR:O	2:F:152:PHE:N	2.52	0.42
2:H:180:GLN:HB3	2:H:180:GLN:HE21	1.62	0.42
2:H:280:PRO:HB3	2:H:288:ARG:CG	2.48	0.42
1:C:335:ASN:HD22	1:C:336:SER:N	2.13	0.42
1:D:310:ILE:HA	1:D:313:PHE:CE2	2.54	0.42
2:H:219:THR:HB	2:H:228:PHE:O	2.19	0.42
1:A:275:GLN:NE2	1:A:278:THR:HG21	2.33	0.42
1:C:400:LEU:HD23	1:C:415:PHE:HE1	1.84	0.42
1:D:306:ASN:O	1:D:310:ILE:HG13	2.19	0.42
2:E:312:ARG:O	2:E:313:LEU:HB3	2.19	0.42
2:F:344:GLU:O	2:F:345:GLU:C	2.57	0.42
3:M:746:ARG:CG	3:M:746:ARG:NH1	2.82	0.42
1:B:306:ASN:N	1:B:306:ASN:HD22	2.14	0.42
2:E:150:TYR:O	2:E:152:PHE:N	2.52	0.42
2:E:346:LEU:HA	2:E:349:MET:HE2	2.01	0.42
2:G:148:PRO:HD2	2:G:151:LEU:HD22	2.01	0.42
2:H:313:LEU:HD23	2:H:314:GLN:N	2.34	0.42
1:B:320:VAL:CG2	1:B:321:LYS:N	2.82	0.42
2:F:212:LEU:C	2:F:212:LEU:HD23	2.39	0.42
2:F:245:GLN:O	2:F:249:LEU:HD22	2.19	0.42
2:G:179:VAL:O	2:G:183:ILE:HG13	2.20	0.42
1:B:310:ILE:HA	1:B:313:PHE:CE2	2.55	0.42
1:C:287:PRO:O	1:C:288:HIS:HB2	2.19	0.42
1:D:285:ARG:HH11	1:D:285:ARG:HG2	1.84	0.42
2:E:146:ARG:N	2:E:146:ARG:HD2	2.35	0.42
2:F:150:TYR:HA	2:F:153:MET:HE3	2.01	0.42
2:F:179:VAL:O	2:F:183:ILE:HG13	2.20	0.42
1:D:366:GLU:CG	1:D:418:LEU:HD21	2.47	0.42
2:E:313:LEU:HD23	2:E:314:GLN:N	2.35	0.42
2:F:146:ARG:HD2	2:F:146:ARG:N	2.35	0.42
1:A:407:LYS:HE2	1:B:233:GLU:CG	2.50	0.42
1:D:321:LYS:HG3	1:D:322:ASP:N	2.35	0.42
2:E:209:VAL:HB	2:E:333:ASN:ND2	2.35	0.42
2:E:197:MET:HE1	3:M:749:LEU:HD12	2.01	0.42
3:M:750:ASP:OD1	3:M:750:ASP:N	2.51	0.42
1:A:406:HIS:NE2	1:B:233:GLU:C	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:306:ASN:HD22	1:C:306:ASN:N	2.15	0.42
2:E:311:SER:O	2:E:312:ARG:CB	2.67	0.42
2:E:324:GLY:O	2:E:327:ALA:HB3	2.19	0.42
1:B:342:VAL:C	1:B:343:GLY:O	2.57	0.42
2:F:341:GLN:O	2:F:343:LEU:N	2.53	0.42
2:F:346:LEU:HD12	2:F:346:LEU:HA	1.84	0.42
2:G:245:GLN:O	2:G:249:LEU:HD22	2.19	0.42
2:H:138:LEU:HD12	2:H:139:PHE:N	2.35	0.42
3:P:750:ASP:OD1	3:P:750:ASP:N	2.51	0.42
1:D:243:GLU:CB	1:D:244:PRO:C	2.81	0.41
2:E:329:LEU:HA	2:E:329:LEU:HD12	1.72	0.41
2:E:342:ARG:HD2	2:E:342:ARG:HH11	1.72	0.41
2:E:344:GLU:O	2:E:345:GLU:C	2.58	0.41
2:G:146:ARG:N	2:G:146:ARG:HD2	2.35	0.41
2:F:281:ASP:N	2:F:281:ASP:OD1	2.52	0.41
2:F:282:ARG:O	2:F:285:VAL:HG13	2.21	0.41
2:H:311:SER:O	2:H:312:ARG:CB	2.68	0.41
1:A:321:LYS:HG3	1:A:322:ASP:N	2.35	0.41
1:A:381:LYS:NZ	2:E:250:GLU:OE1	2.53	0.41
2:E:353:LEU:HA	2:E:353:LEU:HD23	1.88	0.41
2:F:170:HIS:O	2:F:174:ILE:HG12	2.20	0.41
2:F:343:LEU:O	2:F:345:GLU:HG2	2.20	0.41
2:G:209:VAL:O	2:G:212:LEU:HB3	2.20	0.41
1:A:276:LEU:HA	1:A:276:LEU:HD12	1.90	0.41
1:C:276:LEU:HA	1:C:276:LEU:HD12	1.91	0.41
1:C:436:LEU:HD12	1:C:436:LEU:HA	1.91	0.41
1:D:383:LEU:HD12	1:D:383:LEU:HA	1.83	0.41
3:O:751:LYS:HB2	3:O:751:LYS:HE3	1.96	0.41
1:A:387:ALA:O	1:A:390:GLU:HB3	2.20	0.41
1:C:275:GLN:NE2	1:C:278:THR:HG21	2.36	0.41
2:F:138:LEU:HD12	2:F:139:PHE:N	2.35	0.41
2:H:179:VAL:O	2:H:183:ILE:HG13	2.21	0.41
1:C:231:PRO:C	1:C:233:GLU:H	2.24	0.41
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.56	0.41
1:D:416:ALA:HB1	2:H:319:TYR:CZ	2.55	0.41
2:E:220:PHE:O	2:E:260:LYS:HE2	2.20	0.41
2:E:221:CYS:O	2:E:225:GLU:N	2.52	0.41
2:E:294:LEU:O	2:E:298:MET:HB2	2.21	0.41
2:G:192:PHE:C	2:G:194:SER:H	2.24	0.41
2:H:146:ARG:N	2:H:146:ARG:HD2	2.36	0.41
2:H:236:MET:H	2:H:236:MET:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:343:LEU:O	2:H:345:GLU:HG2	2.21	0.41
3:N:751:LYS:HB2	3:N:751:LYS:HE3	1.96	0.41
1:A:301:LEU:HA	1:A:301:LEU:HD23	1.92	0.41
1:C:321:LYS:HG3	1:C:322:ASP:N	2.35	0.41
2:E:138:LEU:HD12	2:E:139:PHE:N	2.36	0.41
2:G:183:ILE:O	2:G:184:LYS:C	2.59	0.41
2:H:318:LEU:HD13	2:H:318:LEU:C	2.40	0.41
2:H:341:GLN:O	2:H:343:LEU:N	2.53	0.41
1:B:400:LEU:HD23	1:B:415:PHE:HE1	1.86	0.41
1:D:315:HIS:CG	1:D:367:LEU:HD22	2.56	0.41
2:H:356:ILE:CD1	3:P:745:LEU:HD21	2.51	0.41
1:A:345:ILE:CD1	1:A:432:CYS:SG	3.08	0.41
1:B:276:LEU:HD12	1:B:276:LEU:HA	1.92	0.41
2:E:201:ILE:HG23	3:M:745:LEU:HD13	2.02	0.41
2:E:280:PRO:HB3	2:E:288:ARG:CG	2.50	0.41
1:A:406:HIS:HE2	1:B:233:GLU:HA	1.71	0.41
1:B:366:GLU:CG	1:B:418:LEU:HD21	2.49	0.41
1:C:299:ILE:HG21	1:C:383:LEU:CD1	2.44	0.41
1:C:305:TRP:CD1	1:C:454:MET:HE2	2.56	0.41
1:D:236:LEU:HG	1:D:365:THR:OG1	2.21	0.41
1:D:320:VAL:CG2	1:D:321:LYS:N	2.84	0.41
2:G:346:LEU:HA	2:G:349:MET:CE	2.51	0.41
2:H:344:GLU:O	2:H:345:GLU:C	2.59	0.41
1:C:342:VAL:C	1:C:343:GLY:O	2.58	0.41
4:D:804:9CR:H10	4:D:804:9CR:H8	1.80	0.41
2:E:197:MET:O	2:E:201:ILE:HG12	2.21	0.41
2:G:204:LEU:HA	2:G:204:LEU:HD12	1.83	0.41
2:E:246:TYR:HB2	2:G:237:GLU:HG2	2.02	0.41
1:A:409:PRO:HD2	1:A:410:GLU:OE2	2.21	0.40
2:E:197:MET:HE1	3:M:749:LEU:CB	2.48	0.40
1:A:416:ALA:HB1	2:E:319:TYR:CE2	2.56	0.40
2:F:279:SER:HA	2:F:280:PRO:HD3	1.82	0.40
2:G:240:VAL:HG23	2:G:241:HIS:N	2.36	0.40
2:G:344:GLU:O	2:G:345:GLU:C	2.59	0.40
2:H:197:MET:CE	3:P:749:LEU:CD1	2.98	0.40
3:I:740:LYS:HE2	3:I:740:LYS:CA	2.43	0.40
3:K:740:LYS:HE2	3:K:740:LYS:CA	2.44	0.40
3:O:749:LEU:HD23	3:O:749:LEU:HA	1.80	0.40
1:A:383:LEU:HA	1:A:383:LEU:HD12	1.83	0.40
1:A:430:LEU:HD11	2:E:331:SER:HA	2.02	0.40
1:B:383:LEU:HD12	1:B:383:LEU:HA	1.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:313:LEU:HD23	2:F:314:GLN:N	2.35	0.40
2:G:138:LEU:HD12	2:G:139:PHE:N	2.36	0.40
1:A:410:GLU:CD	1:A:410:GLU:H	2.23	0.40
1:D:275:GLN:NE2	1:D:278:THR:HG21	2.35	0.40
1:D:345:ILE:O	1:D:349:VAL:HG23	2.21	0.40
2:H:286:THR:O	2:H:288:ARG:N	2.49	0.40
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.56	0.40
1:B:317:SER:OG	1:B:324:ILE:HA	2.22	0.40
1:B:273:ASP:OD1	1:B:449:THR:O	2.40	0.40
1:D:433:LEU:HD23	1:D:433:LEU:HA	1.83	0.40
2:E:280:PRO:HB3	2:E:288:ARG:HG2	2.04	0.40
2:F:197:MET:HE1	3:N:749:LEU:HB2	2.02	0.40
2:F:271:LEU:HA	2:F:271:LEU:HD23	1.94	0.40
2:H:220:PHE:O	2:H:260:LYS:HE2	2.21	0.40
3:L:744:LEU:O	3:L:748:LEU:HG	2.22	0.40
1:A:406:HIS:CD2	1:A:407:LYS:N	2.90	0.40
1:A:447:ILE:O	1:A:447:ILE:CG1	2.65	0.40
2:G:345:GLU:HB2	2:G:349:MET:HE2	2.03	0.40
3:O:741:GLU:HG3	3:O:742:ASN:ND2	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:342:ARG:NH1	2:H:156:ARG:O[1_655]	1.81	0.39
2:F:342:ARG:NH1	2:H:157:PRO:CD[1_655]	1.88	0.32
1:B:442:ILE:O	2:E:161:ARG:NH1[1_554]	2.17	0.03

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/232 (99%)	191 (83%)	26 (11%)	13 (6%)	1	8
1	B	230/232 (99%)	190 (83%)	27 (12%)	13 (6%)	1	8
1	C	230/232 (99%)	191 (83%)	25 (11%)	14 (6%)	1	7
1	D	230/232 (99%)	189 (82%)	27 (12%)	14 (6%)	1	7
2	E	240/242 (99%)	206 (86%)	22 (9%)	12 (5%)	2	10
2	F	240/242 (99%)	207 (86%)	20 (8%)	13 (5%)	2	9
2	G	240/242 (99%)	206 (86%)	21 (9%)	13 (5%)	2	9
2	H	240/242 (99%)	209 (87%)	18 (8%)	13 (5%)	2	9
3	I	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	4
3	J	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	4
3	K	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	4
3	L	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	4
3	M	16/18 (89%)	9 (56%)	3 (19%)	4 (25%)	0	0
3	N	16/18 (89%)	10 (62%)	1 (6%)	5 (31%)	0	0
3	O	16/18 (89%)	10 (62%)	3 (19%)	3 (19%)	0	0
3	P	16/18 (89%)	9 (56%)	4 (25%)	3 (19%)	0	0
All	All	2000/2040 (98%)	1667 (83%)	209 (10%)	124 (6%)	1	6

All (124) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	PRO
1	A	245	LYS
1	A	256	LEU
1	A	260	SER
1	A	261	PRO
1	A	321	LYS
1	B	244	PRO
1	B	245	LYS
1	B	256	LEU
1	B	260	SER
1	B	261	PRO
1	B	321	LYS
1	C	244	PRO
1	C	245	LYS
1	C	256	LEU
1	C	260	SER

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Mol	Chain	Res	Type
1	C	261	PRO
1	C	321	LYS
1	C	449	THR
1	D	244	PRO
1	D	245	LYS
1	D	256	LEU
1	D	260	SER
1	D	261	PRO
1	D	321	LYS
2	E	156	ARG
2	E	310	GLN
2	E	311	SER
2	E	313	LEU
2	E	314	GLN
2	E	316	ARG
2	F	156	ARG
2	F	310	GLN
2	F	311	SER
2	F	313	LEU
2	F	314	GLN
2	F	316	ARG
2	G	156	ARG
2	G	310	GLN
2	G	311	SER
2	G	313	LEU
2	G	314	GLN
2	G	316	ARG
2	G	342	ARG
2	H	156	ARG
2	H	310	GLN
2	H	311	SER
2	H	313	LEU
2	H	314	GLN
2	H	316	ARG
3	I	751	LYS
3	J	751	LYS
3	K	751	LYS
3	L	751	LYS
3	M	754	THR
3	N	754	THR
3	O	754	THR
3	P	754	THR

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Mol	Chain	Res	Type
1	A	247	GLU
1	A	259	SER
1	A	449	THR
1	B	247	GLU
1	B	449	THR
1	C	247	GLU
1	D	247	GLU
1	D	259	SER
1	D	449	THR
2	E	342	ARG
2	F	151	LEU
2	F	342	ARG
2	G	151	LEU
2	H	342	ARG
3	M	741	GLU
3	N	741	GLU
3	O	741	GLU
3	P	741	GLU
1	B	259	SER
1	C	259	SER
1	C	457	ALA
1	D	448	ASP
2	E	151	LEU
2	E	312	ARG
2	E	344	GLU
2	E	345	GLU
2	F	312	ARG
2	F	344	GLU
2	F	345	GLU
2	G	312	ARG
2	G	344	GLU
2	G	345	GLU
2	H	151	LEU
2	H	312	ARG
2	H	344	GLU
2	H	345	GLU
3	M	751	LYS
3	N	751	LYS
3	O	751	LYS
3	P	751	LYS
1	A	444	ASP
1	A	448	ASP

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Mol	Chain	Res	Type
1	A	457	ALA
1	B	444	ASP
1	B	457	ALA
1	C	444	ASP
1	D	444	ASP
1	D	457	ALA
2	E	317	PHE
2	F	317	PHE
2	G	317	PHE
2	H	317	PHE
1	A	257	ASN
1	B	257	ASN
1	B	448	ASP
1	C	257	ASN
1	C	282	TRP
1	C	448	ASP
1	D	257	ASN
1	D	282	TRP
2	H	308	GLU
2	F	308	GLU
2	G	308	GLU
3	M	742	ASN
3	N	740	LYS
3	N	742	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/200 (91%)	163 (90%)	19 (10%)	7	24
1	B	182/200 (91%)	163 (90%)	19 (10%)	7	24
1	C	182/200 (91%)	163 (90%)	19 (10%)	7	24
1	D	182/200 (91%)	163 (90%)	19 (10%)	7	24
2	E	217/217 (100%)	191 (88%)	26 (12%)	5	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	217/217 (100%)	194 (89%)	23 (11%)	6	24
2	G	217/217 (100%)	193 (89%)	24 (11%)	6	22
2	H	217/217 (100%)	193 (89%)	24 (11%)	6	22
3	I	14/16 (88%)	10 (71%)	4 (29%)	0	1
3	J	14/16 (88%)	10 (71%)	4 (29%)	0	1
3	K	14/16 (88%)	10 (71%)	4 (29%)	0	1
3	L	14/16 (88%)	10 (71%)	4 (29%)	0	1
3	M	16/16 (100%)	11 (69%)	5 (31%)	0	1
3	N	16/16 (100%)	11 (69%)	5 (31%)	0	1
3	O	16/16 (100%)	11 (69%)	5 (31%)	0	1
3	P	16/16 (100%)	12 (75%)	4 (25%)	0	2
All	All	1716/1796 (96%)	1508 (88%)	208 (12%)	5	19

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	236	LEU
1	A	278	THR
1	A	294	LEU
1	A	302	ARG
1	A	306	ASN
1	A	313	PHE
1	A	325	LEU
1	A	334	ARG
1	A	335	ASN
1	A	345	ILE
1	A	347	ASP
1	A	383	LEU
1	A	410	GLU
1	A	420	LEU
1	A	436	LEU
1	A	444	ASP
1	A	450	PHE
1	A	455	LEU
1	A	456	GLU
1	B	236	LEU
1	B	278	THR
1	B	294	LEU

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Mol	Chain	Res	Type
1	B	302	ARG
1	B	306	ASN
1	B	313	PHE
1	B	325	LEU
1	B	334	ARG
1	B	335	ASN
1	B	345	ILE
1	B	347	ASP
1	B	383	LEU
1	B	410	GLU
1	B	420	LEU
1	B	436	LEU
1	B	444	ASP
1	B	450	PHE
1	B	455	LEU
1	B	456	GLU
1	C	236	LEU
1	C	278	THR
1	C	294	LEU
1	C	302	ARG
1	C	306	ASN
1	C	313	PHE
1	C	325	LEU
1	C	334	ARG
1	C	335	ASN
1	C	345	ILE
1	C	347	ASP
1	C	383	LEU
1	C	410	GLU
1	C	420	LEU
1	C	436	LEU
1	C	444	ASP
1	C	450	PHE
1	C	455	LEU
1	C	456	GLU
1	D	236	LEU
1	D	278	THR
1	D	294	LEU
1	D	302	ARG
1	D	306	ASN
1	D	313	PHE
1	D	325	LEU

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Mol	Chain	Res	Type
1	D	334	ARG
1	D	335	ASN
1	D	345	ILE
1	D	347	ASP
1	D	383	LEU
1	D	410	GLU
1	D	420	LEU
1	D	436	LEU
1	D	444	ASP
1	D	450	PHE
1	D	455	LEU
1	D	456	GLU
2	E	123	LEU
2	E	135	VAL
2	E	138	LEU
2	E	146	ARG
2	E	150	TYR
2	E	151	LEU
2	E	156	ARG
2	E	168	LEU
2	E	197	MET
2	E	198	GLU
2	E	236	MET
2	E	237	GLU
2	E	249	LEU
2	E	250	GLU
2	E	251	SER
2	E	253	LEU
2	E	277	LEU
2	E	282	ARG
2	E	302	LEU
2	E	303	ASN
2	E	316	ARG
2	E	329	LEU
2	E	330	ARG
2	E	345	GLU
2	E	353	LEU
2	E	355	GLU
2	F	123	LEU
2	F	135	VAL
2	F	138	LEU
2	F	146	ARG

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Mol	Chain	Res	Type
2	F	150	TYR
2	F	151	LEU
2	F	156	ARG
2	F	168	LEU
2	F	198	GLU
2	F	236	MET
2	F	237	GLU
2	F	250	GLU
2	F	251	SER
2	F	277	LEU
2	F	282	ARG
2	F	302	LEU
2	F	303	ASN
2	F	316	ARG
2	F	329	LEU
2	F	330	ARG
2	F	345	GLU
2	F	353	LEU
2	F	355	GLU
2	G	123	LEU
2	G	135	VAL
2	G	138	LEU
2	G	146	ARG
2	G	150	TYR
2	G	151	LEU
2	G	156	ARG
2	G	168	LEU
2	G	236	MET
2	G	237	GLU
2	G	250	GLU
2	G	251	SER
2	G	253	LEU
2	G	277	LEU
2	G	282	ARG
2	G	302	LEU
2	G	303	ASN
2	G	316	ARG
2	G	329	LEU
2	G	330	ARG
2	G	342	ARG
2	G	345	GLU
2	G	353	LEU

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Mol	Chain	Res	Type
2	G	355	GLU
2	H	123	LEU
2	H	135	VAL
2	H	138	LEU
2	H	146	ARG
2	H	150	TYR
2	H	151	LEU
2	H	156	ARG
2	H	168	LEU
2	H	198	GLU
2	H	236	MET
2	H	237	GLU
2	H	250	GLU
2	H	251	SER
2	H	253	LEU
2	H	277	LEU
2	H	282	ARG
2	H	302	LEU
2	H	303	ASN
2	H	316	ARG
2	H	329	LEU
2	H	330	ARG
2	H	345	GLU
2	H	353	LEU
2	H	355	GLU
3	I	742	ASN
3	I	745	LEU
3	I	750	ASP
3	I	752	ASP
3	J	742	ASN
3	J	745	LEU
3	J	750	ASP
3	J	752	ASP
3	K	742	ASN
3	K	745	LEU
3	K	750	ASP
3	K	752	ASP
3	L	742	ASN
3	L	745	LEU
3	L	750	ASP
3	L	752	ASP
3	M	740	LYS

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Mol	Chain	Res	Type
3	M	744	LEU
3	M	746	ARG
3	M	751	LYS
3	M	754	THR
3	N	740	LYS
3	N	746	ARG
3	N	750	ASP
3	N	751	LYS
3	N	754	THR
3	O	740	LYS
3	O	744	LEU
3	O	750	ASP
3	O	751	LYS
3	O	754	THR
3	P	740	LYS
3	P	746	ARG
3	P	751	LYS
3	P	754	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	A	306	ASN
1	A	335	ASN
1	B	270	GLN
1	B	306	ASN
1	B	331	HIS
1	B	335	ASN
1	B	406	HIS
1	C	270	GLN
1	C	306	ASN
1	C	331	HIS
1	C	335	ASN
1	C	406	HIS
1	D	270	GLN
1	D	306	ASN
1	D	335	ASN
2	E	120	GLN
2	E	125	GLN
2	E	141	GLN
2	E	144	GLN

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Mol	Chain	Res	Type
2	E	159	GLN
2	E	175	ASN
2	E	180	GLN
2	E	181	GLN
2	E	245	GLN
2	E	258	ASN
2	E	303	ASN
2	E	314	GLN
2	E	333	ASN
2	E	341	GLN
2	F	120	GLN
2	F	125	GLN
2	F	141	GLN
2	F	144	GLN
2	F	159	GLN
2	F	175	ASN
2	F	180	GLN
2	F	181	GLN
2	F	245	GLN
2	F	254	HIS
2	F	258	ASN
2	F	314	GLN
2	F	333	ASN
2	F	341	GLN
2	G	120	GLN
2	G	125	GLN
2	G	141	GLN
2	G	144	GLN
2	G	159	GLN
2	G	175	ASN
2	G	181	GLN
2	G	245	GLN
2	G	254	HIS
2	G	258	ASN
2	G	263	HIS
2	G	314	GLN
2	G	333	ASN
2	G	341	GLN
2	H	120	GLN
2	H	125	GLN
2	H	141	GLN
2	H	144	GLN

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Mol	Chain	Res	Type
2	H	159	GLN
2	H	175	ASN
2	H	180	GLN
2	H	181	GLN
2	H	200	GLN
2	H	245	GLN
2	H	258	ASN
2	H	303	ASN
2	H	314	GLN
2	H	333	ASN
2	H	341	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	9CR	C	803	-	19,22,22	4.33	12 (63%)	26,30,30	2.92	14 (53%)
5	TCD	H	808	-	24,26,26	2.14	4 (16%)	28,36,36	1.98	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	9CR	B	802	-	19,22,22	4.25	12 (63%)	26,30,30	2.90	13 (50%)
5	TCD	E	805	-	24,26,26	2.41	4 (16%)	28,36,36	1.96	8 (28%)
4	9CR	A	801	-	19,22,22	4.22	12 (63%)	26,30,30	2.90	12 (46%)
5	TCD	F	806	-	24,26,26	2.21	3 (12%)	28,36,36	1.88	6 (21%)
4	9CR	D	804	-	19,22,22	4.30	13 (68%)	26,30,30	2.90	12 (46%)
5	TCD	G	807	-	24,26,26	2.46	5 (20%)	28,36,36	1.92	8 (28%)

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
4	9CR	C	803	-	-	2/13/32/32	0/1/1/1
5	TCD	H	808	-	-	0/8/8/8	0/3/3/3
4	9CR	B	802	-	-	2/13/32/32	0/1/1/1
5	TCD	E	805	-	-	0/8/8/8	0/3/3/3
4	9CR	A	801	-	-	2/13/32/32	0/1/1/1
5	TCD	F	806	-	-	0/8/8/8	0/3/3/3
4	9CR	D	804	-	-	2/13/32/32	0/1/1/1
5	TCD	G	807	-	-	0/8/8/8	0/3/3/3

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	9CR	C1-C6	10.36	1.68	1.53
4	D	804	9CR	C1-C6	10.31	1.67	1.53
4	B	802	9CR	C1-C6	10.06	1.67	1.53
5	G	807	TCD	C26-C27	9.98	1.54	1.38
4	A	801	9CR	C1-C6	9.86	1.67	1.53
4	C	803	9CR	C5-C6	9.76	1.51	1.34
5	E	805	TCD	C26-C27	9.76	1.54	1.38
4	D	804	9CR	C5-C6	9.43	1.50	1.34
4	A	801	9CR	C5-C6	9.37	1.50	1.34
4	B	802	9CR	C5-C6	9.37	1.50	1.34
5	F	806	TCD	C26-C27	8.24	1.51	1.38
5	H	808	TCD	C26-C27	7.99	1.51	1.38
4	B	802	9CR	C14-C13	5.55	1.41	1.35
4	A	801	9CR	C14-C13	5.40	1.41	1.35
4	D	804	9CR	C14-C13	5.32	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	803	9CR	C14-C13	5.31	1.41	1.35
4	A	801	9CR	C4-C5	-4.99	1.41	1.51
4	D	804	9CR	C4-C5	-4.91	1.41	1.51
4	B	802	9CR	C4-C5	-4.88	1.41	1.51
4	C	803	9CR	C4-C5	-4.66	1.41	1.51
4	D	804	9CR	C19-C9	4.26	1.59	1.50
4	A	801	9CR	C19-C9	4.24	1.59	1.50
4	C	803	9CR	C19-C9	4.11	1.59	1.50
4	B	802	9CR	C19-C9	4.08	1.59	1.50
4	C	803	9CR	C2-C1	3.87	1.63	1.54
4	D	804	9CR	C2-C1	3.80	1.62	1.54
4	B	802	9CR	C2-C1	3.75	1.62	1.54
4	A	801	9CR	C2-C1	3.74	1.62	1.54
4	D	804	9CR	C3-C4	-3.70	1.40	1.52
4	C	803	9CR	C10-C9	3.67	1.40	1.35
4	A	801	9CR	C3-C4	-3.66	1.40	1.52
4	B	802	9CR	C3-C4	-3.57	1.40	1.52
4	C	803	9CR	C3-C4	-3.49	1.40	1.52
5	E	805	TCD	C22-N23	3.49	1.39	1.32
4	B	802	9CR	C10-C9	3.41	1.40	1.35
5	F	806	TCD	C36-C35	3.40	1.43	1.38
4	D	804	9CR	C2-C3	3.37	1.60	1.52
4	C	803	9CR	C2-C3	3.35	1.60	1.52
5	H	808	TCD	C36-C35	3.34	1.43	1.38
4	A	801	9CR	C2-C3	3.30	1.60	1.52
4	B	802	9CR	C2-C3	3.21	1.60	1.52
4	D	804	9CR	C16-C1	3.17	1.60	1.53
4	D	804	9CR	C10-C9	3.10	1.39	1.35
4	A	801	9CR	C10-C9	3.09	1.39	1.35
4	C	803	9CR	C16-C1	2.99	1.59	1.53
4	B	802	9CR	C16-C1	2.97	1.59	1.53
5	F	806	TCD	C34-C35	2.97	1.45	1.38
4	B	802	9CR	C8-C9	-2.97	1.39	1.45
4	A	801	9CR	C16-C1	2.96	1.59	1.53
4	C	803	9CR	C8-C9	-2.89	1.39	1.45
4	A	801	9CR	C8-C9	-2.81	1.39	1.45
5	G	807	TCD	C22-N23	2.78	1.37	1.32
4	D	804	9CR	C8-C9	-2.72	1.40	1.45
5	G	807	TCD	C32-N33	2.59	1.37	1.32
5	H	808	TCD	C34-C35	2.43	1.43	1.38
4	D	804	9CR	C20-C13	2.32	1.55	1.50
4	C	803	9CR	C20-C13	2.31	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	805	TCD	O31-C4	-2.21	1.34	1.39
4	B	802	9CR	C20-C13	2.21	1.55	1.50
5	H	808	TCD	C22-N23	2.15	1.36	1.32
4	A	801	9CR	C20-C13	2.13	1.55	1.50
5	E	805	TCD	C36-C35	2.05	1.41	1.38
5	G	807	TCD	C36-C35	2.04	1.41	1.38
4	D	804	9CR	C8-C7	2.01	1.39	1.33
5	G	807	TCD	C3-C4	2.00	1.42	1.38

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	9CR	C19-C9-C10	-6.00	114.52	122.92
4	D	804	9CR	C19-C9-C10	-6.00	114.52	122.92
4	C	803	9CR	C19-C9-C10	-5.97	114.56	122.92
4	B	802	9CR	C19-C9-C10	-5.97	114.56	122.92
4	B	802	9CR	C1-C6-C5	-5.36	115.06	122.61
4	C	803	9CR	C1-C6-C5	-5.33	115.10	122.61
4	D	804	9CR	C1-C6-C5	-5.31	115.13	122.61
4	A	801	9CR	C1-C6-C5	-5.28	115.18	122.61
5	H	808	TCD	C36-C35-C34	-5.15	115.36	119.96
4	A	801	9CR	C17-C1-C6	4.80	118.09	110.30
4	C	803	9CR	C17-C1-C6	4.70	117.92	110.30
5	F	806	TCD	C36-C35-C34	-4.69	115.77	119.96
5	E	805	TCD	C36-C35-C34	-4.66	115.80	119.96
4	B	802	9CR	C17-C1-C6	4.66	117.85	110.30
4	D	804	9CR	C17-C1-C6	4.61	117.78	110.30
4	C	803	9CR	C7-C8-C9	4.54	133.09	126.23
4	D	804	9CR	C7-C8-C9	4.51	133.05	126.23
4	A	801	9CR	C7-C8-C9	4.46	132.97	126.23
4	B	802	9CR	C7-C8-C9	4.44	132.95	126.23
4	C	803	9CR	C20-C13-C12	4.38	124.98	118.08
4	B	802	9CR	C20-C13-C12	4.33	124.89	118.08
4	D	804	9CR	C19-C9-C8	4.30	124.86	118.08
4	A	801	9CR	C19-C9-C8	4.28	124.82	118.08
4	C	803	9CR	C3-C4-C5	4.27	121.70	114.08
4	D	804	9CR	C20-C13-C12	4.23	124.74	118.08
4	C	803	9CR	C19-C9-C8	4.22	124.72	118.08
4	B	802	9CR	C19-C9-C8	4.21	124.71	118.08
5	G	807	TCD	C36-C35-C34	-4.21	116.20	119.96
4	A	801	9CR	C20-C13-C12	4.18	124.67	118.08
4	B	802	9CR	C3-C4-C5	4.15	121.48	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	804	9CR	C3-C4-C5	4.14	121.48	114.08
4	A	801	9CR	C3-C4-C5	4.05	121.31	114.08
4	D	804	9CR	C11-C10-C9	-3.71	122.02	127.31
4	A	801	9CR	C11-C10-C9	-3.65	122.11	127.31
5	F	806	TCD	O21-C22-N23	-3.59	114.73	119.49
5	F	806	TCD	C26-C25-C24	-3.55	116.78	119.96
5	H	808	TCD	O21-C22-N23	-3.55	114.78	119.49
4	B	802	9CR	C11-C10-C9	-3.53	122.28	127.31
5	G	807	TCD	C26-C25-C24	-3.51	116.82	119.96
5	G	807	TCD	O21-C22-N23	-3.48	114.88	119.49
5	E	805	TCD	O21-C22-N23	-3.44	114.92	119.49
4	C	803	9CR	C11-C10-C9	-3.44	122.39	127.31
5	H	808	TCD	C26-C25-C24	-3.43	116.89	119.96
5	G	807	TCD	C37-C36-C35	3.41	122.53	118.71
5	E	805	TCD	C4-O31-C32	3.23	124.54	118.16
4	D	804	9CR	C8-C7-C6	2.97	135.54	127.20
5	E	805	TCD	C37-C36-C35	2.97	122.03	118.71
5	H	808	TCD	C36-C35-CL35	2.95	122.84	119.15
4	A	801	9CR	C8-C7-C6	2.95	135.47	127.20
5	G	807	TCD	C4-O31-C32	2.92	123.93	118.16
4	C	803	9CR	C8-C7-C6	2.91	135.38	127.20
4	B	802	9CR	C8-C7-C6	2.86	135.24	127.20
5	E	805	TCD	C26-C25-C24	-2.84	117.42	119.96
5	F	806	TCD	C36-C35-CL35	2.78	122.63	119.15
5	H	808	TCD	O31-C32-N33	2.65	123.00	119.49
4	B	802	9CR	C12-C13-C14	-2.56	112.26	119.11
4	C	803	9CR	C12-C13-C14	-2.52	112.39	119.11
4	A	801	9CR	C12-C13-C14	-2.51	112.41	119.11
5	E	805	TCD	C36-C35-CL35	2.51	122.28	119.15
4	D	804	9CR	C12-C13-C14	-2.50	112.42	119.11
5	G	807	TCD	C24-N23-C22	2.49	122.68	116.27
5	H	808	TCD	C24-N23-C22	2.49	122.67	116.27
5	F	806	TCD	C24-N23-C22	2.46	122.58	116.27
5	G	807	TCD	C27-C26-C25	2.44	121.44	118.71
5	E	805	TCD	C24-N23-C22	2.41	122.47	116.27
5	E	805	TCD	C27-C26-C25	2.39	121.39	118.71
4	A	801	9CR	C16-C1-C6	-2.34	106.50	110.30
4	C	803	9CR	C18-C5-C6	2.34	127.16	124.53
4	B	802	9CR	C16-C1-C6	-2.34	106.51	110.30
4	C	803	9CR	C16-C1-C6	-2.28	106.59	110.30
4	B	802	9CR	C18-C5-C6	2.25	127.05	124.53
5	G	807	TCD	C36-C35-CL35	2.21	121.91	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	804	9CR	C16-C1-C6	-2.17	106.79	110.30
4	B	802	9CR	C2-C1-C6	2.12	113.74	110.48
4	D	804	9CR	C18-C5-C6	2.09	126.87	124.53
4	C	803	9CR	C2-C1-C6	2.07	113.67	110.48
5	H	808	TCD	C34-N33-C32	2.05	121.53	116.27
4	A	801	9CR	C18-C5-C6	2.04	126.81	124.53
5	F	806	TCD	C4-O31-C32	2.01	122.14	118.16
4	C	803	9CR	C7-C6-C5	2.00	126.31	121.46

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	803	9CR	C11-C10-C9-C19
4	B	802	9CR	C11-C10-C9-C19
4	A	801	9CR	C11-C10-C9-C19
4	D	804	9CR	C11-C10-C9-C19
4	C	803	9CR	C11-C10-C9-C8
4	B	802	9CR	C11-C10-C9-C8
4	A	801	9CR	C11-C10-C9-C8
4	D	804	9CR	C11-C10-C9-C8

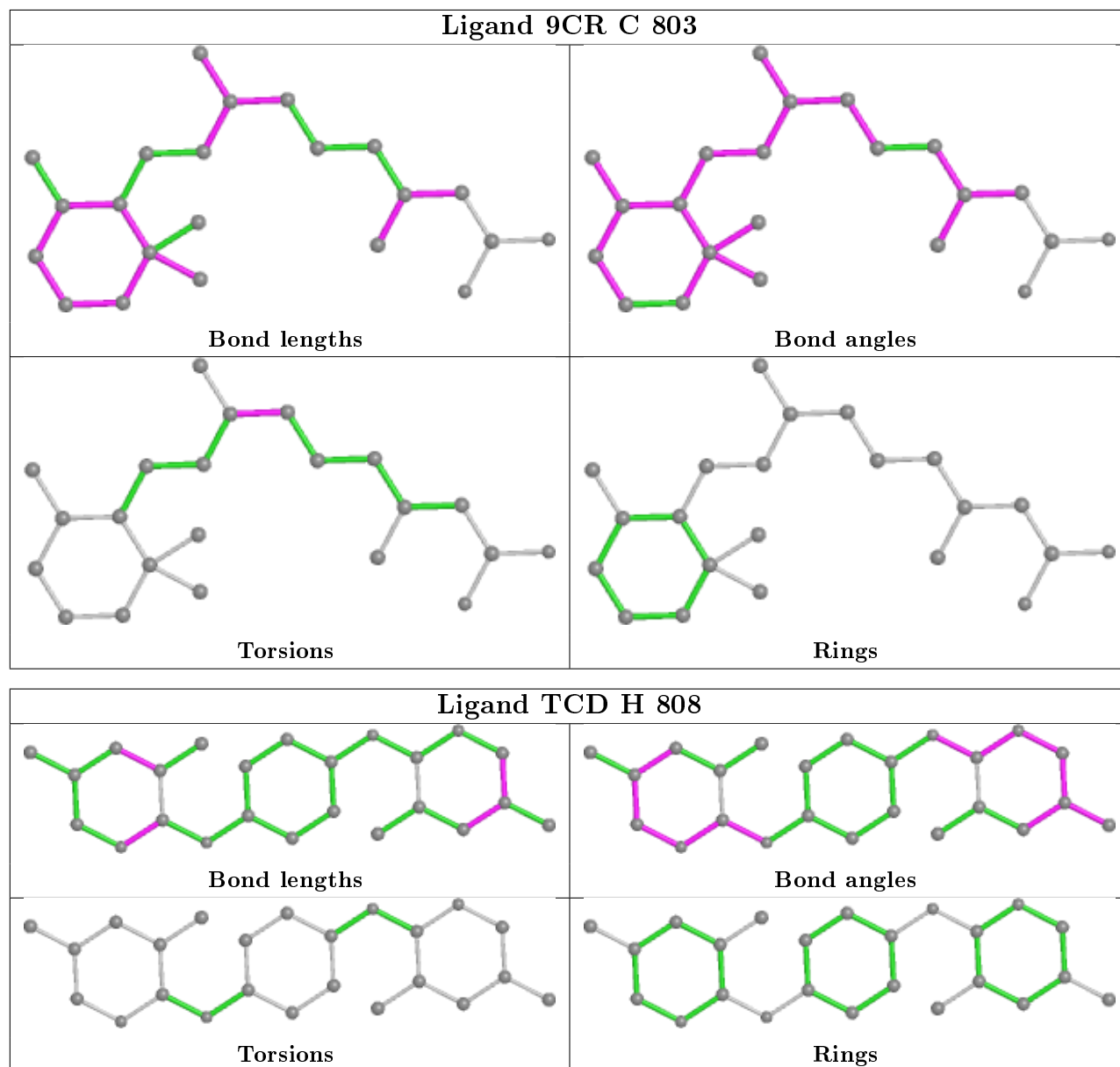
There are no ring outliers.

8 monomers are involved in 18 short contacts:

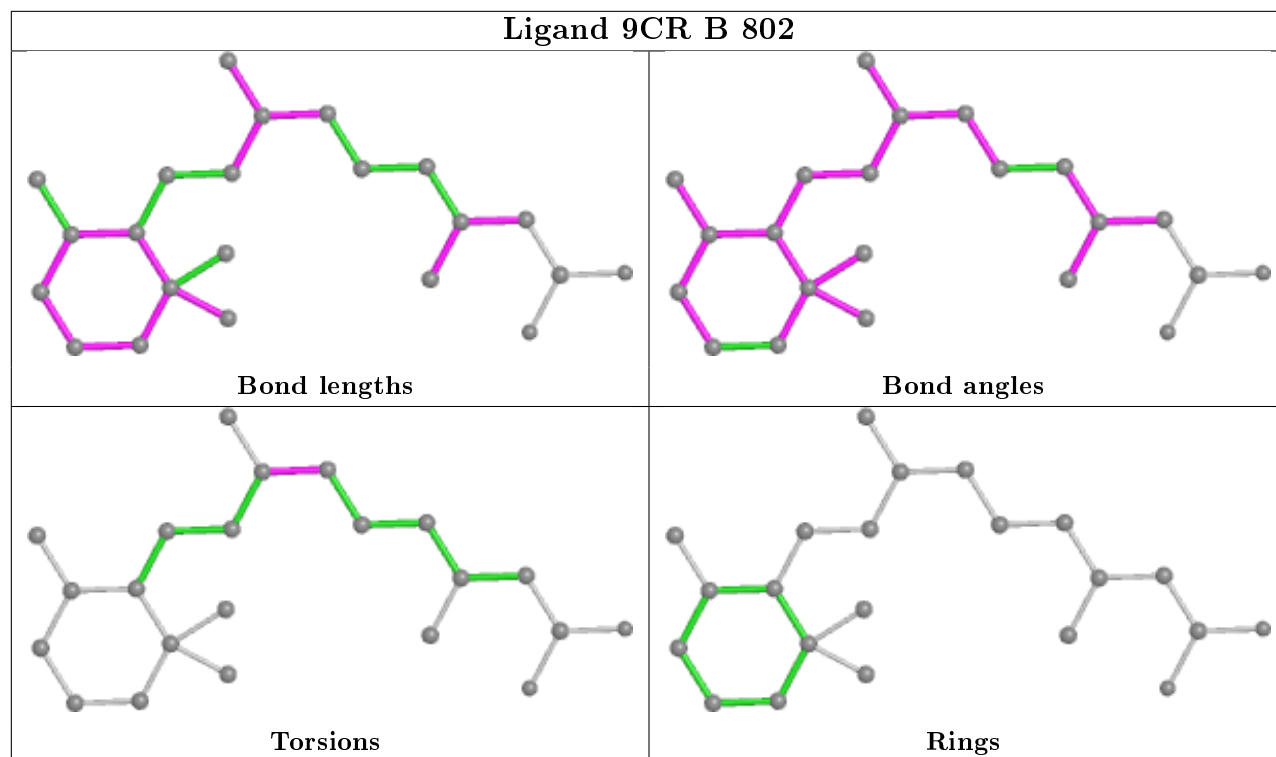
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	803	9CR	4	0
5	H	808	TCD	1	0
4	B	802	9CR	3	0
5	E	805	TCD	1	0
4	A	801	9CR	3	0
5	F	806	TCD	1	0
4	D	804	9CR	4	0
5	G	807	TCD	1	0

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 than 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

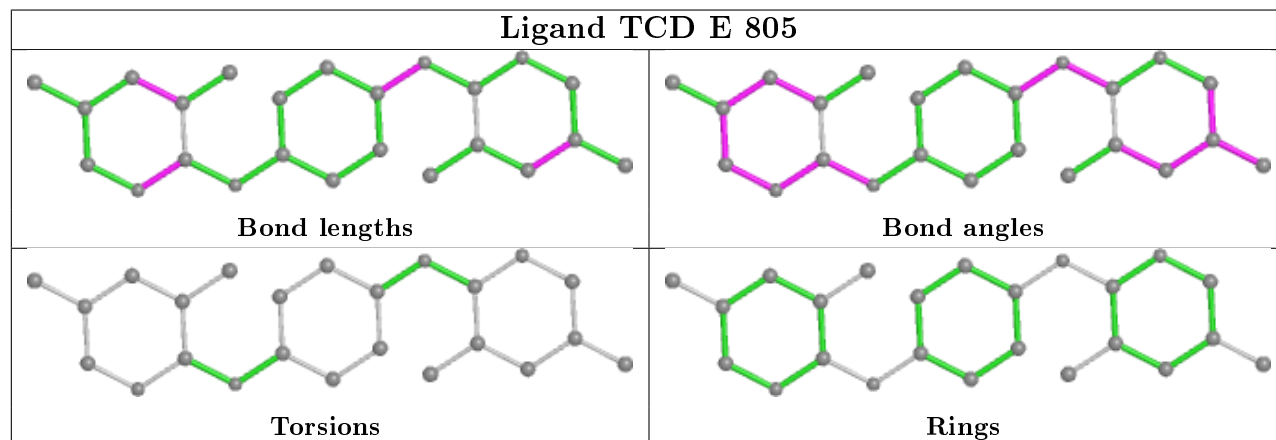
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

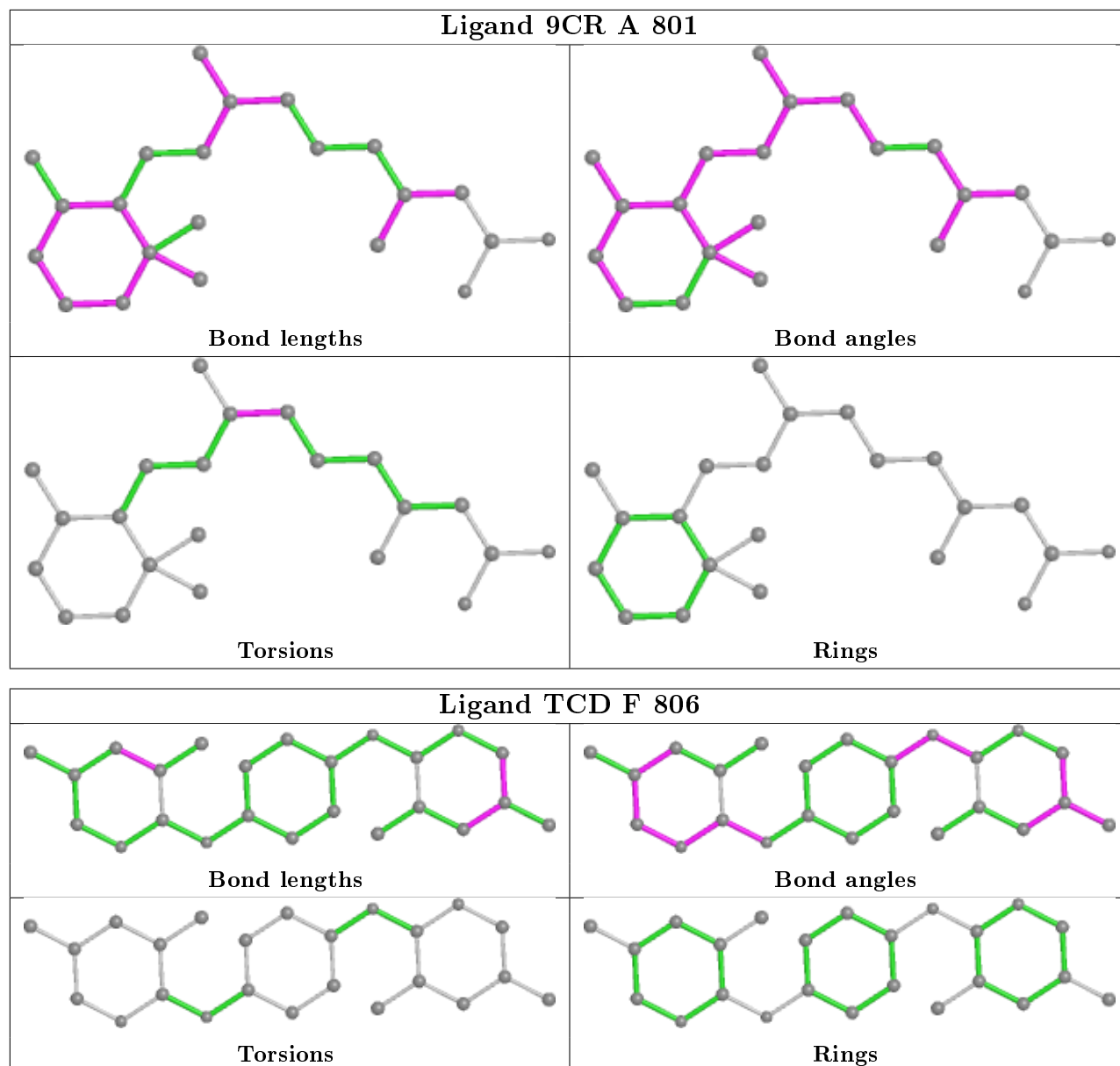


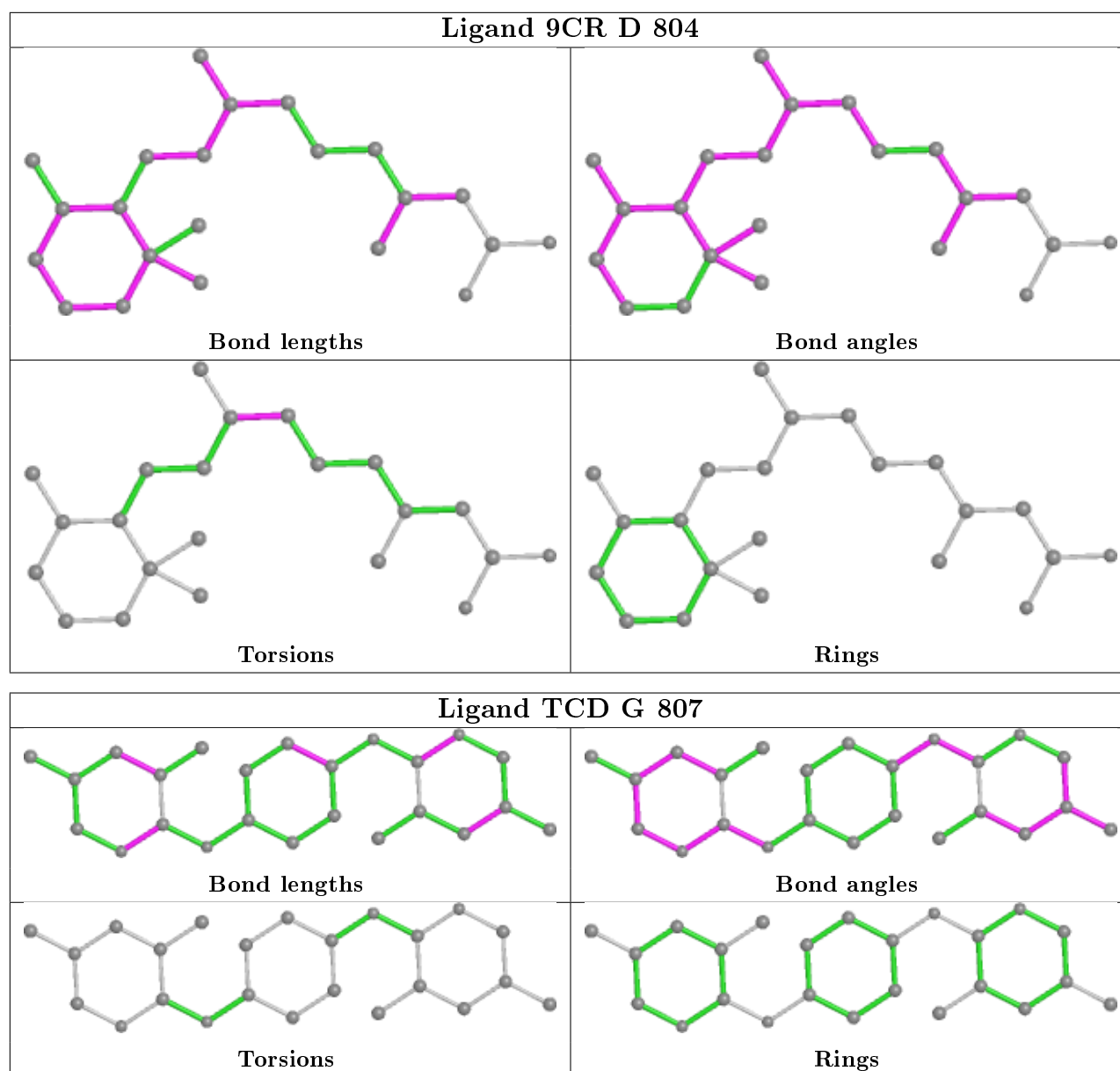
Ligand 9CR B 802



Ligand TCD E 805







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	232/232 (100%)	0.42	24 (10%) 6 4	22, 47, 126, 134	0
1	B	232/232 (100%)	0.54	26 (11%) 5 3	22, 50, 128, 137	0
1	C	232/232 (100%)	0.56	26 (11%) 5 3	21, 53, 127, 136	0
1	D	232/232 (100%)	0.42	21 (9%) 9 5	21, 50, 125, 135	0
2	E	242/242 (100%)	-0.05	11 (4%) 33 21	21, 44, 89, 122	0
2	F	242/242 (100%)	0.09	13 (5%) 25 16	16, 42, 89, 127	0
2	G	242/242 (100%)	0.14	19 (7%) 12 7	17, 44, 88, 126	0
2	H	242/242 (100%)	-0.01	15 (6%) 20 12	18, 44, 89, 121	0
3	I	16/18 (88%)	1.40	4 (25%) 0 0	43, 79, 130, 135	0
3	J	16/18 (88%)	2.42	6 (37%) 0 0	51, 82, 132, 134	0
3	K	16/18 (88%)	2.32	7 (43%) 0 0	53, 85, 134, 136	0
3	L	16/18 (88%)	1.24	5 (31%) 0 0	43, 77, 131, 137	0
3	M	18/18 (100%)	0.95	1 (5%) 24 15	37, 77, 121, 125	0
3	N	18/18 (100%)	1.68	7 (38%) 0 0	39, 76, 121, 129	0
3	O	18/18 (100%)	1.38	5 (27%) 0 0	39, 75, 120, 129	0
3	P	18/18 (100%)	0.91	4 (22%) 0 0	37, 80, 120, 124	0
All	All	2032/2040 (99%)	0.34	194 (9%) 8 5	16, 48, 120, 137	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	TYR	13.7
1	B	248	THR	13.6
1	C	255	GLY	12.4
3	K	754	THR	11.2
1	D	252	ALA	10.4

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Mol	Chain	Res	Type	RSRZ
1	D	254	MET	10.3
1	D	251	GLU	10.3
1	B	249	TYR	10.1
2	G	161	ARG	9.9
1	A	250	VAL	9.7
3	J	753	ASP	9.3
1	C	254	MET	9.1
1	C	248	THR	8.9
3	O	739	ALA	8.9
1	B	255	GLY	8.8
1	C	457	ALA	8.7
3	J	754	THR	8.7
1	D	248	THR	8.6
1	D	260	SER	8.6
1	B	254	MET	8.5
1	D	249	TYR	8.5
1	B	253	ASN	8.3
3	K	753	ASP	8.1
1	C	256	LEU	8.1
1	C	458	PRO	8.0
1	B	256	LEU	7.9
2	F	161	ARG	7.9
1	B	247	GLU	7.6
3	J	752	ASP	7.5
2	G	162	GLY	7.3
1	B	458	PRO	7.3
1	C	257	ASN	7.3
1	D	247	GLU	7.2
1	A	253	ASN	7.2
2	F	162	GLY	7.1
1	D	253	ASN	7.1
1	B	262	ASN	7.0
3	I	739	ALA	7.0
1	A	252	ALA	7.0
3	N	739	ALA	6.9
1	B	246	THR	6.8
3	L	739	ALA	6.8
2	F	160	PRO	6.7
1	C	247	GLU	6.6
1	C	260	SER	6.6
1	A	257	ASN	6.5
3	K	752	ASP	6.5

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Mol	Chain	Res	Type	RSRZ
3	J	739	ALA	6.3
3	L	754	THR	6.0
1	B	257	ASN	5.9
1	B	252	ALA	5.8
2	G	157	PRO	5.6
1	A	258	PRO	5.6
1	A	260	SER	5.6
1	B	261	PRO	5.5
2	G	154	HIS	5.4
1	C	251	GLU	5.3
1	D	250	VAL	5.3
2	G	159	GLN	5.3
3	N	740	LYS	5.2
1	A	254	MET	5.2
2	G	160	PRO	5.2
2	F	159	GLN	5.2
1	C	262	ASN	5.2
1	A	244	PRO	5.2
1	A	458	PRO	5.0
1	B	245	LYS	5.0
3	I	754	THR	4.9
1	A	251	GLU	4.9
1	D	257	ASN	4.9
1	C	261	PRO	4.8
3	P	756	ASP	4.8
1	C	252	ALA	4.8
1	B	260	SER	4.7
2	H	310	GLN	4.7
3	N	756	ASP	4.7
3	O	756	ASP	4.7
2	F	157	PRO	4.7
2	E	312	ARG	4.6
2	G	312	ARG	4.6
3	K	739	ALA	4.5
1	A	245	LYS	4.5
3	L	741	GLU	4.4
3	I	753	ASP	4.4
2	G	313	LEU	4.4
1	C	444	ASP	4.4
2	G	342	ARG	4.3
1	C	249	TYR	4.3
1	B	457	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
3	M	756	ASP	4.3
1	B	250	VAL	4.2
2	E	310	GLN	4.2
1	C	229	ASP	4.1
1	D	246	THR	4.1
2	H	161	ARG	4.1
1	D	335	ASN	4.0
1	B	251	GLU	4.0
2	F	312	ARG	4.0
2	E	342	ARG	3.9
3	P	742	ASN	3.9
1	B	243	GLU	3.9
1	C	253	ASN	3.9
2	H	160	PRO	3.7
1	C	227	ASN	3.7
2	E	358	SER	3.7
3	O	754	THR	3.7
1	A	248	THR	3.5
1	D	458	PRO	3.5
3	N	755	LYS	3.5
1	C	246	THR	3.4
1	D	227	ASN	3.4
2	F	311	SER	3.4
2	F	154	HIS	3.4
2	G	314	GLN	3.4
1	C	245	LYS	3.4
1	B	227	ASN	3.4
2	F	163	PRO	3.3
1	D	258	PRO	3.3
2	G	158	PHE	3.3
2	G	163	PRO	3.2
2	H	312	ARG	3.2
2	H	311	SER	3.1
1	A	255	GLY	3.1
1	D	322	ASP	3.1
2	G	310	GLN	3.1
2	H	155	HIS	3.1
2	E	160	PRO	3.1
2	E	316	ARG	3.0
1	C	442	ILE	3.0
2	H	342	ARG	2.9
3	N	750	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	133	ARG	2.8
2	G	311	SER	2.8
2	H	316	ARG	2.8
1	A	338	HIS	2.8
3	J	741	GLU	2.8
3	L	753	ASP	2.8
2	E	158	PHE	2.7
1	A	243	GLU	2.7
1	A	261	PRO	2.7
2	G	316	ARG	2.7
1	B	258	PRO	2.7
3	I	752	ASP	2.7
1	D	244	PRO	2.6
1	A	334	ARG	2.6
2	E	161	ARG	2.6
2	F	158	PHE	2.6
1	D	255	GLY	2.6
3	N	754	THR	2.5
3	O	740	LYS	2.5
2	H	358	SER	2.5
3	K	740	LYS	2.5
2	E	311	SER	2.5
3	O	755	LYS	2.5
1	C	242	VAL	2.5
1	A	227	ASN	2.5
2	F	156	ARG	2.5
1	C	456	GLU	2.5
2	F	313	LEU	2.4
2	E	155	HIS	2.4
1	A	256	LEU	2.3
1	D	261	PRO	2.3
1	A	246	THR	2.3
1	A	369	CYS	2.3
2	E	157	PRO	2.3
1	A	247	GLU	2.3
1	B	228	GLU	2.3
2	H	117	ASN	2.3
1	D	240	LEU	2.3
1	C	250	VAL	2.2
1	C	322	ASP	2.2
2	H	118	GLN	2.2
2	F	316	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	158	PHE	2.2
3	K	741	GLU	2.2
2	G	247	GLU	2.2
2	G	156	ARG	2.2
1	D	406	HIS	2.2
1	C	443	GLY	2.1
2	G	155	HIS	2.1
3	J	740	LYS	2.1
2	G	198	GLU	2.1
2	H	236	MET	2.1
3	P	750	ASP	2.1
3	L	752	ASP	2.1
1	B	244	PRO	2.1
3	K	750	ASP	2.1
3	P	752	ASP	2.1
1	B	340	ALA	2.1
1	B	268	ILE	2.0
3	N	753	ASP	2.0
1	B	446	PRO	2.0
1	A	268	ILE	2.0
2	H	132	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

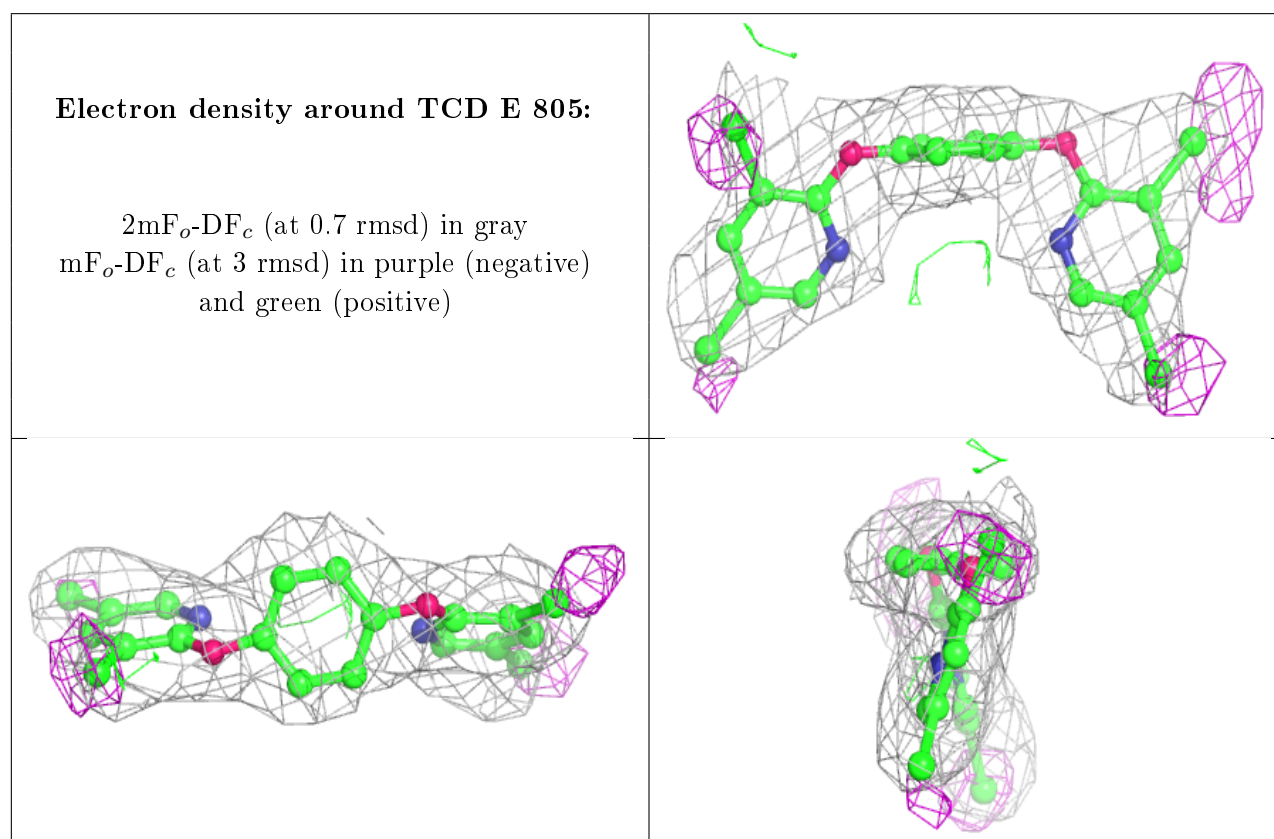
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	TCD	E	805	24/24	0.82	0.30	27,42,54,54	0
5	TCD	H	808	24/24	0.83	0.26	27,37,54,54	0

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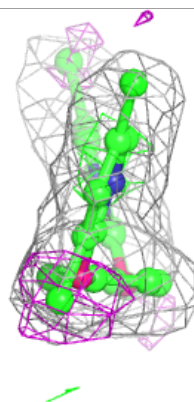
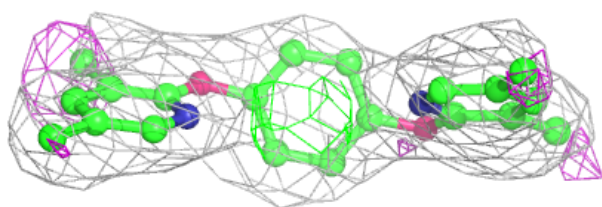
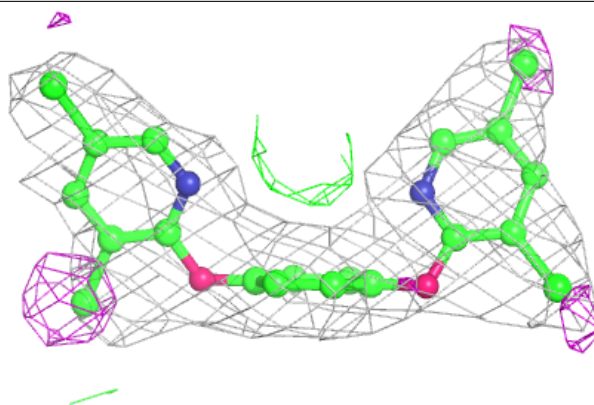
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	9CR	C	803	22/22	0.87	0.26	32,41,48,48	0
5	TCD	G	807	24/24	0.88	0.23	12,38,54,54	0
4	9CR	B	802	22/22	0.90	0.28	26,36,41,47	0
5	TCD	F	806	24/24	0.92	0.19	14,35,54,54	0
4	9CR	A	801	22/22	0.92	0.38	31,43,48,53	0
4	9CR	D	804	22/22	0.93	0.33	31,39,44,49	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.

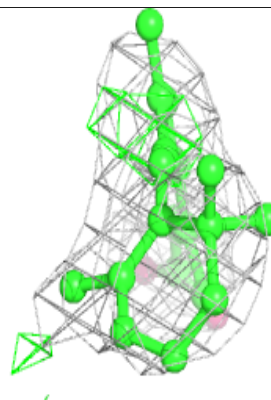
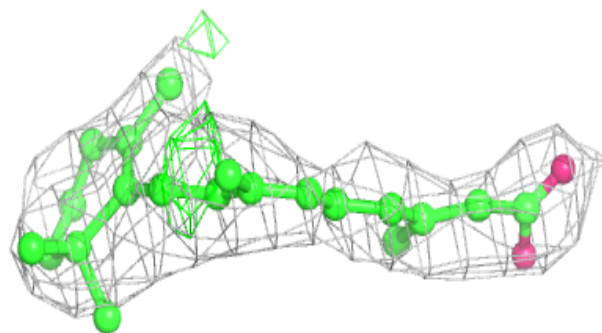
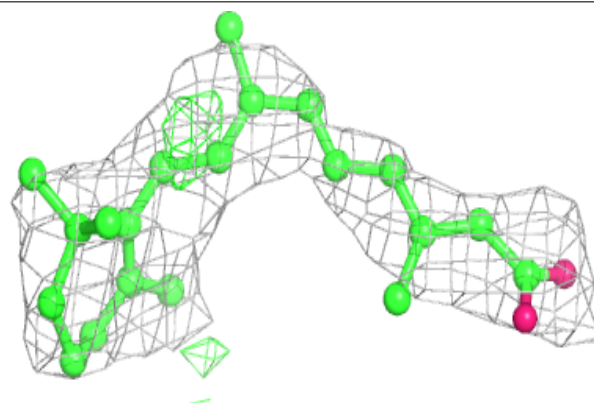


Electron density around TCD H 808:

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

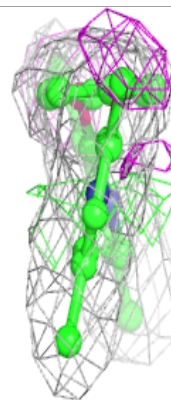
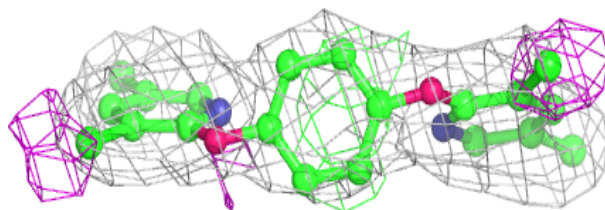
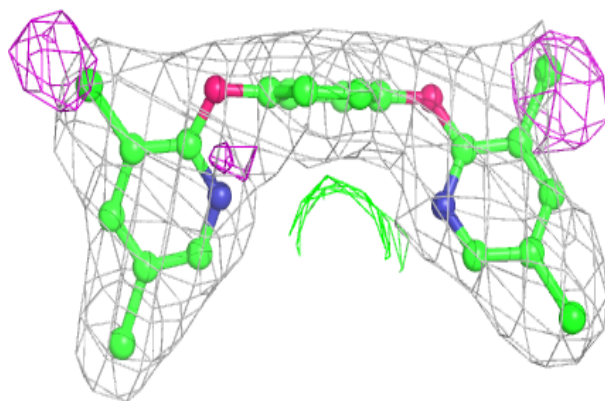
**Electron density around 9CR C 803:**

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

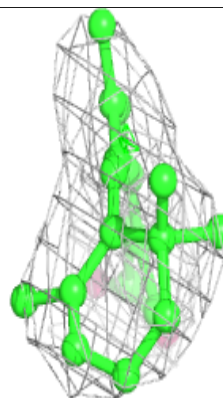
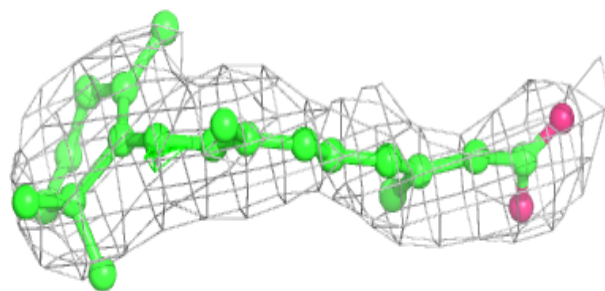
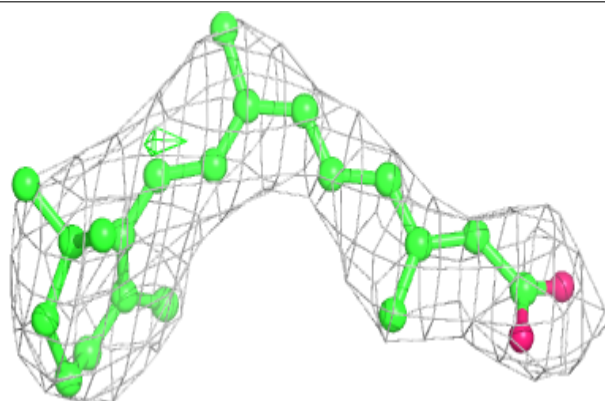


Electron density around TCD G 807:

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

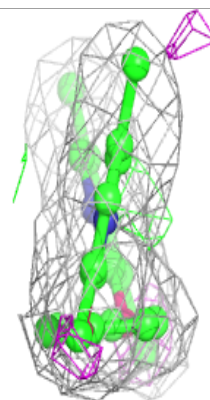
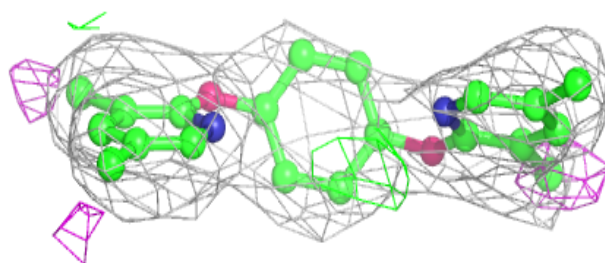
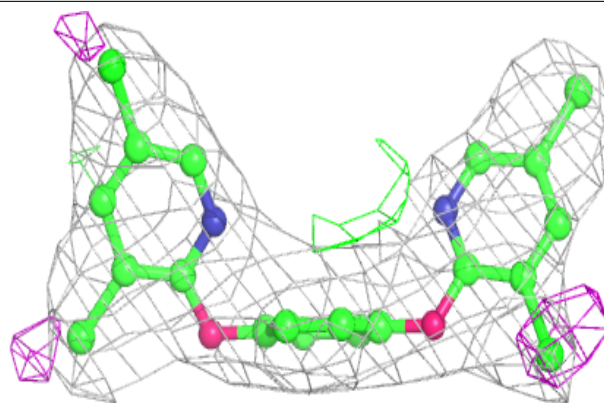
**Electron density around 9CR B 802:**

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

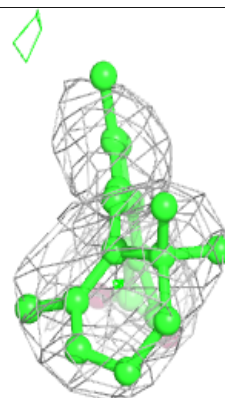
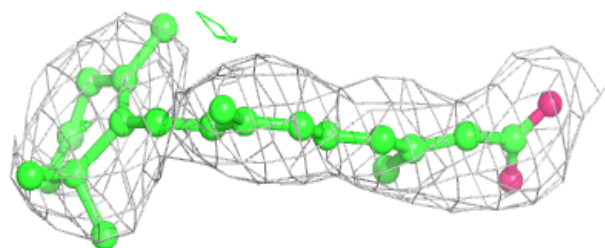
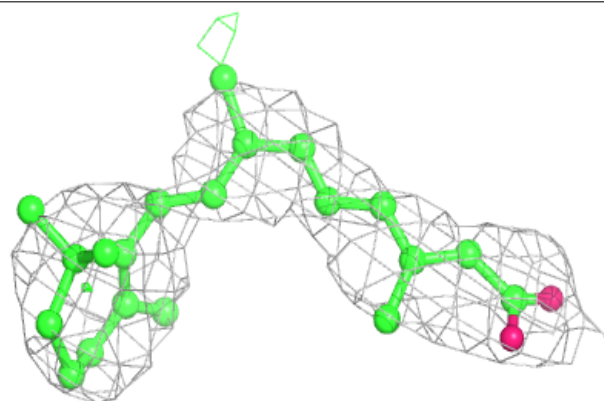


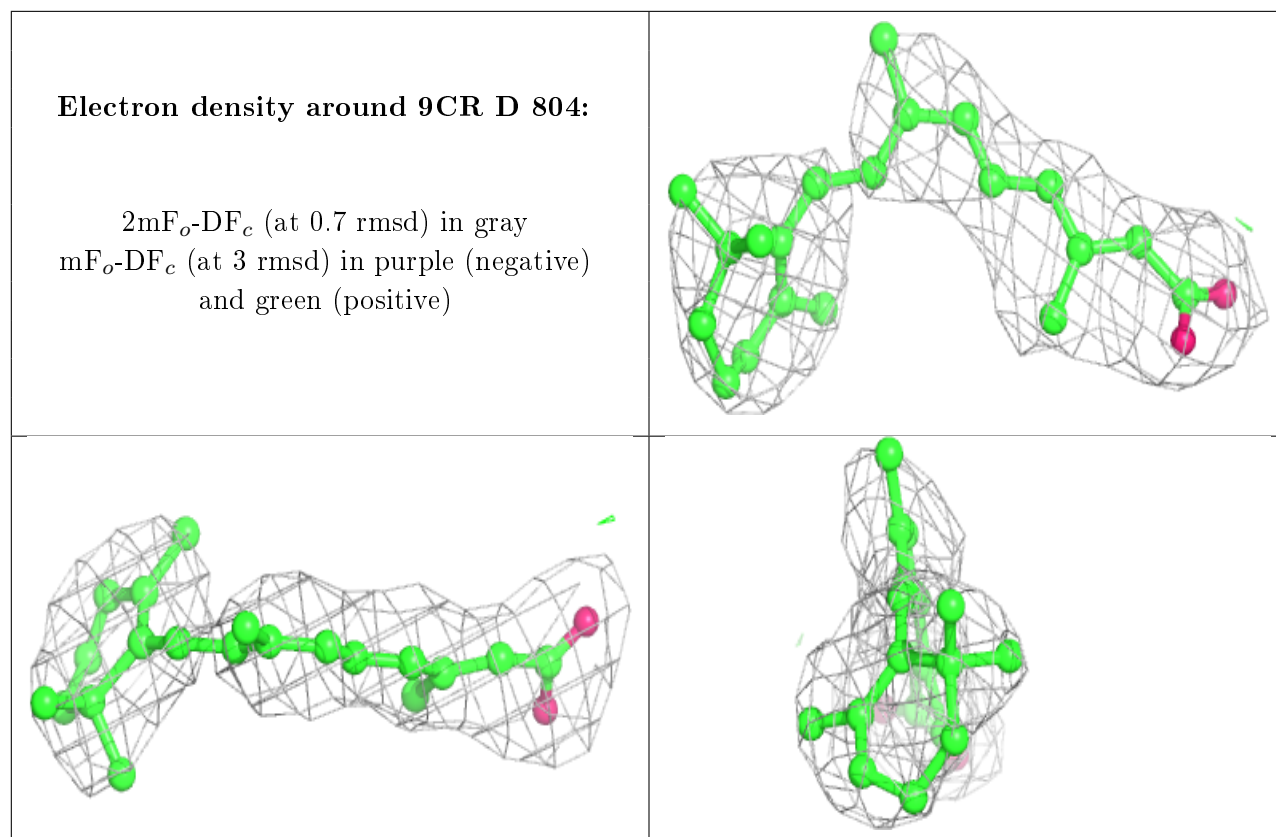
Electron density around TCD F 806:

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

**Electron density around 9CR A 801:**

$2mF_o-DF_c$ (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.