



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2016 – 04:35 PM EDT

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

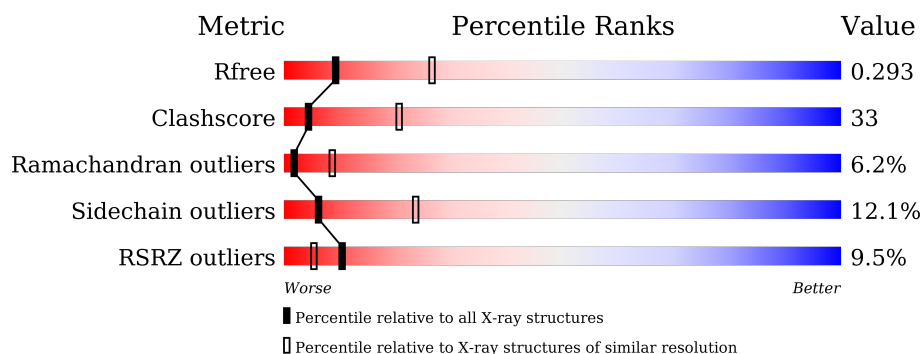
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	<div> <div>10%</div> <div>56%</div> <div>35%</div> <div>8%</div> </div>
1	B	232	<div> <div>11%</div> <div>55%</div> <div>37%</div> <div>8%</div> </div>
1	C	232	<div> <div>11%</div> <div>57%</div> <div>34%</div> <div>9%</div> </div>
1	D	232	<div> <div>9%</div> <div>56%</div> <div>34%</div> <div>9%</div> </div>
2	E	242	<div> <div>5%</div> <div>44%</div> <div>43%</div> <div>10%</div> <div>.</div> </div>
2	F	242	<div> <div>6%</div> <div>47%</div> <div>42%</div> <div>9%</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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	9CR	A	801	-	-	-	X
4	9CR	D	804	-	-	-	X
5	TCD	E	805	-	-	-	X
5	TCD	H	808	-	-	-	X

## 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

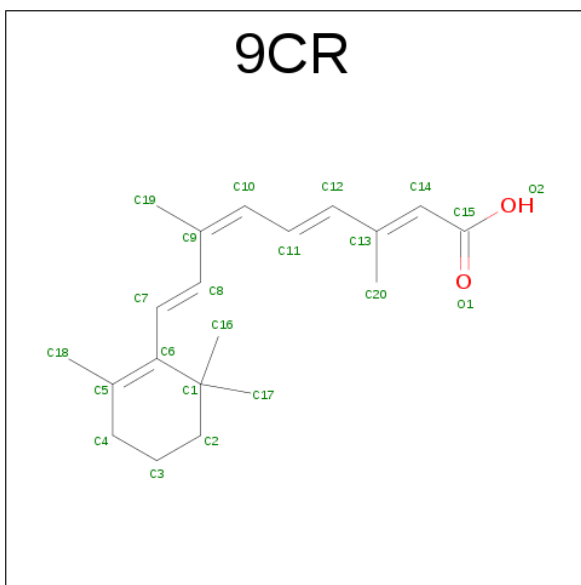
- Molecule 3 is a protein called Nuclear receptor coactivator 2.

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:

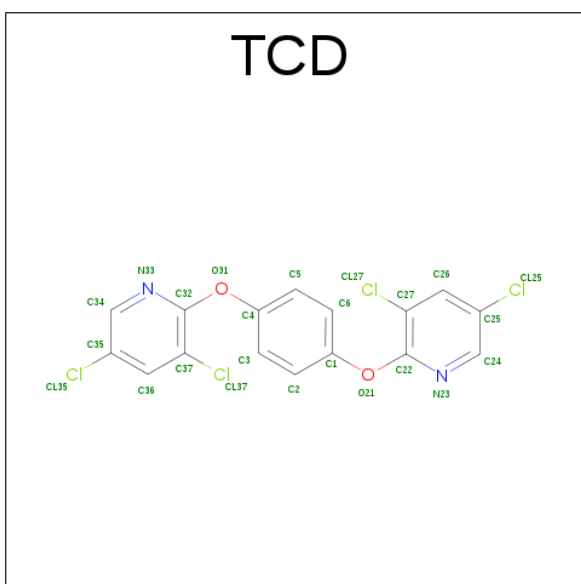
Chain	Residue	Modelled	Actual	Comment	Reference
I	739	ALA	LYS	CONFLICT	UNP Q9WUI9
J	739	ALA	LYS	CONFLICT	UNP Q9WUI9
K	739	ALA	LYS	CONFLICT	UNP Q9WUI9
L	739	ALA	LYS	CONFLICT	UNP Q9WUI9
M	739	ALA	LYS	CONFLICT	UNP Q9WUI9
N	739	ALA	LYS	CONFLICT	UNP Q9WUI9
O	739	ALA	LYS	CONFLICT	UNP Q9WUI9
P	739	ALA	LYS	CONFLICT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

- Molecule 4 is (9CIS)-RETINOIC ACID (three-letter code: 9CR) (formula: C<sub>20</sub>H<sub>28</sub>O<sub>2</sub>).



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		

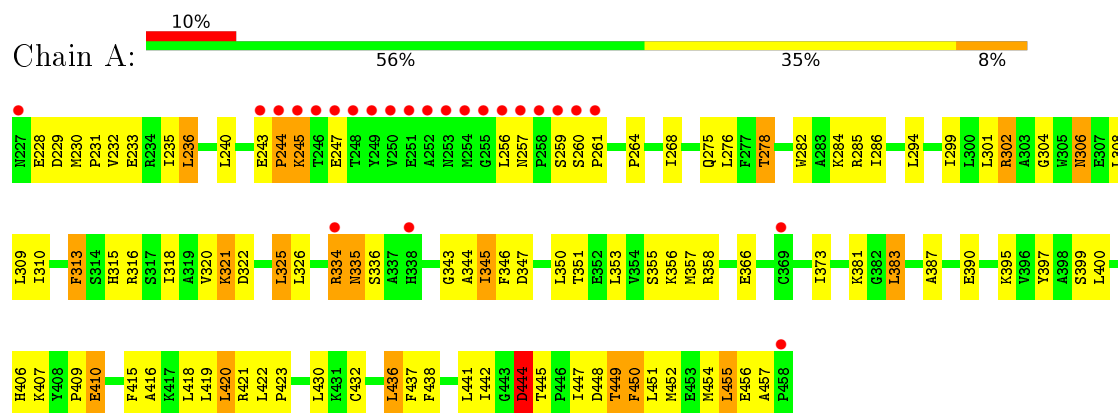
- Molecule 6 is water.

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		

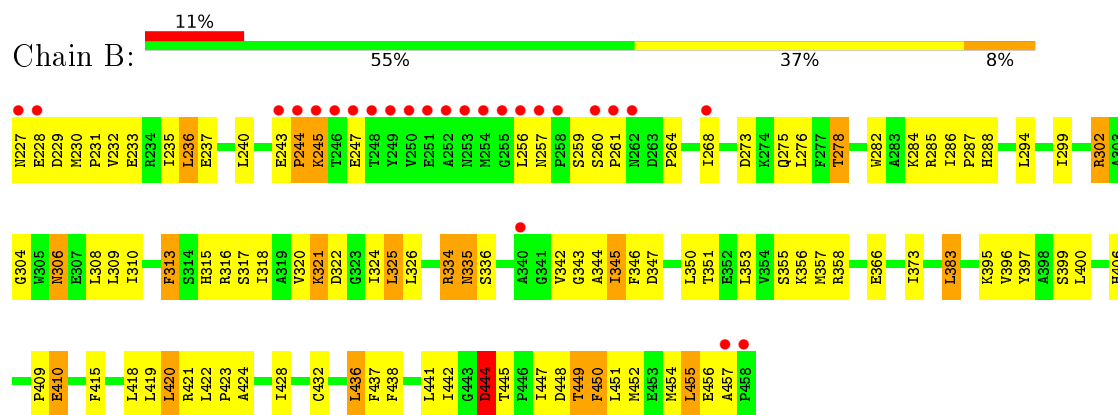
### 3 Residue-property plots

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

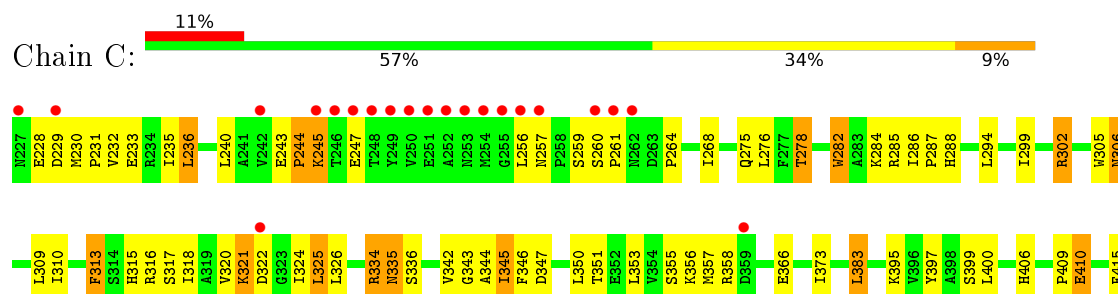
#### • Molecule 1: Retinoic acid receptor RXR-alpha



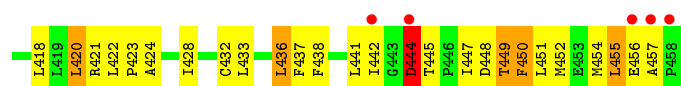
#### • Molecule 1: Retinoic acid receptor RXR-alpha



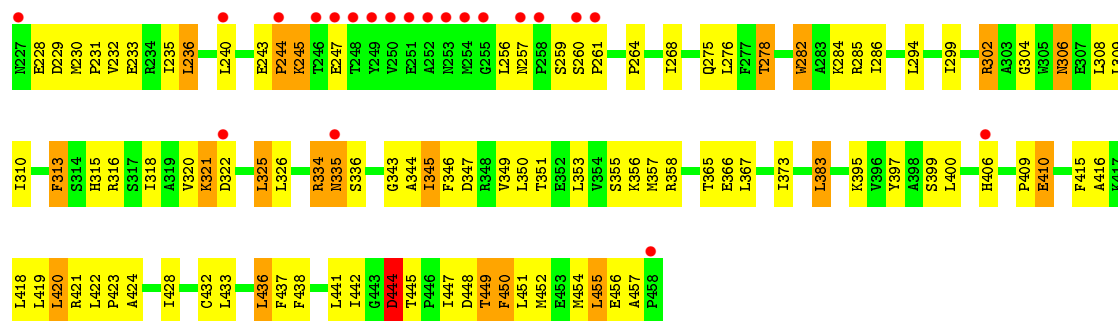
#### • Molecule 1: Retinoic acid receptor RXR-alpha



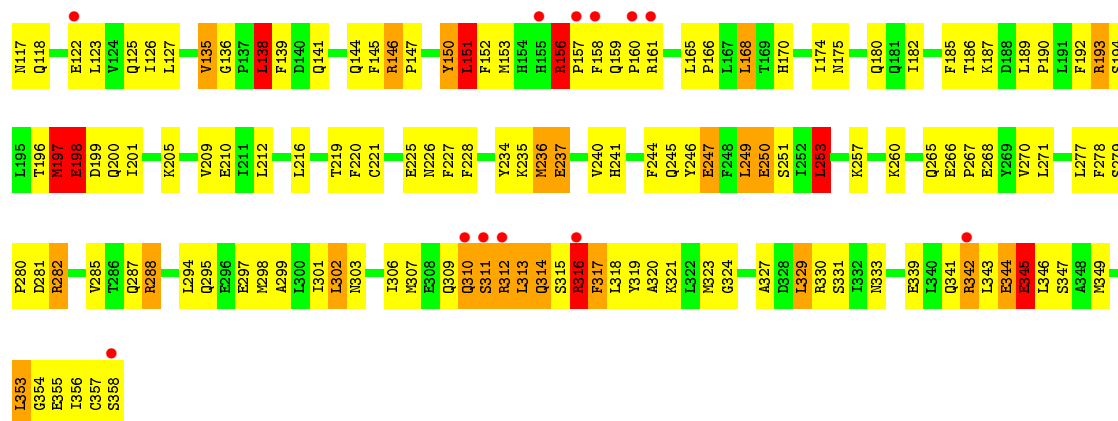
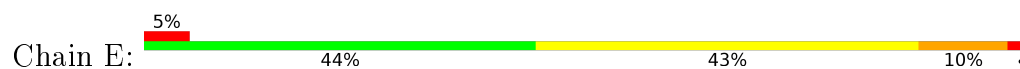




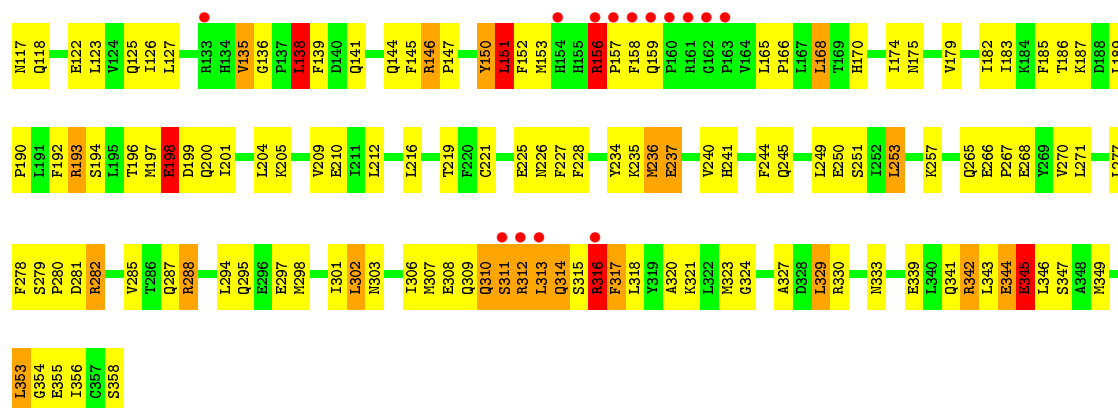
• Molecule 1: Retinoic acid receptor RXR-alpha



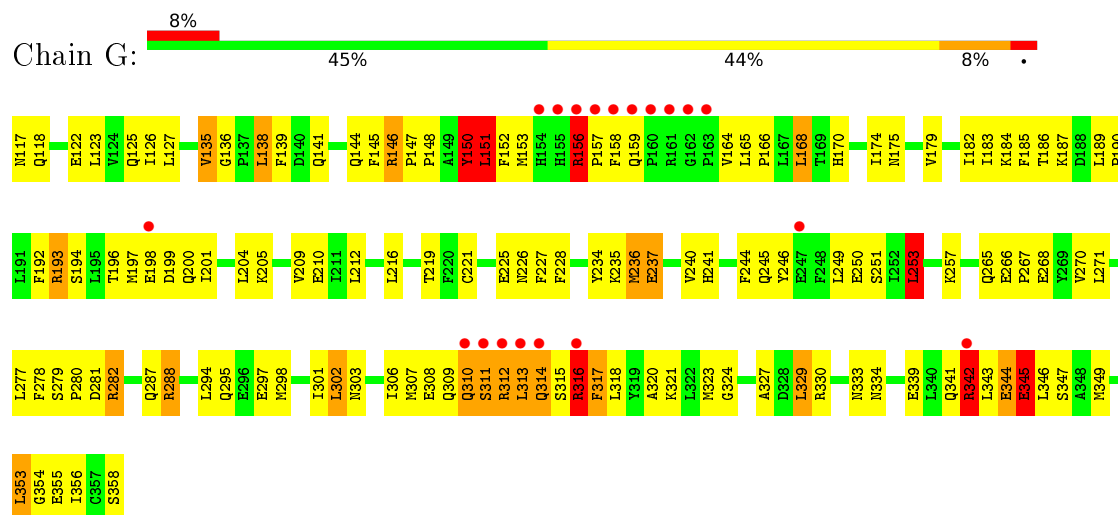
• Molecule 2: Orphan nuclear receptor NR1I3



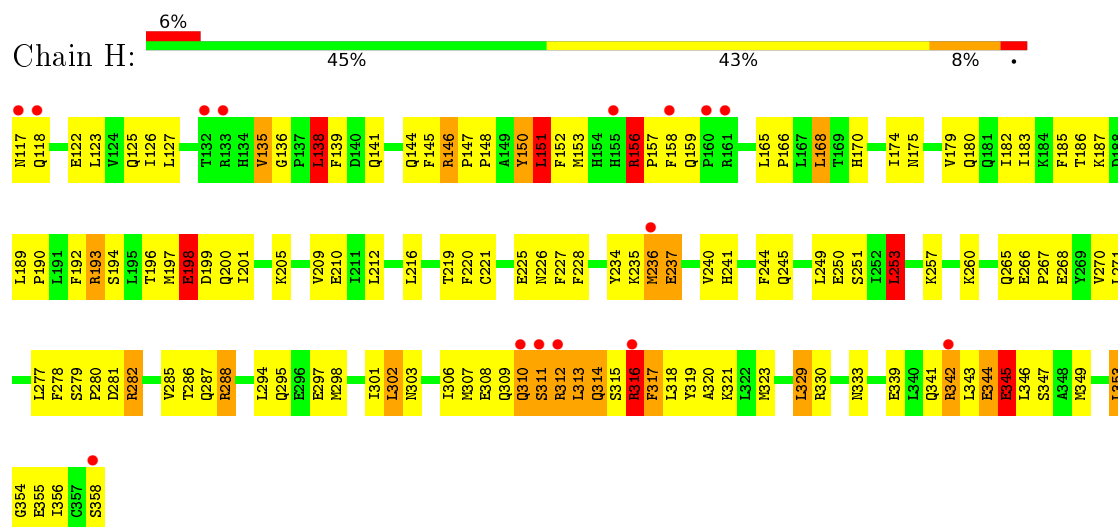
• Molecule 2: Orphan nuclear receptor NR1I3



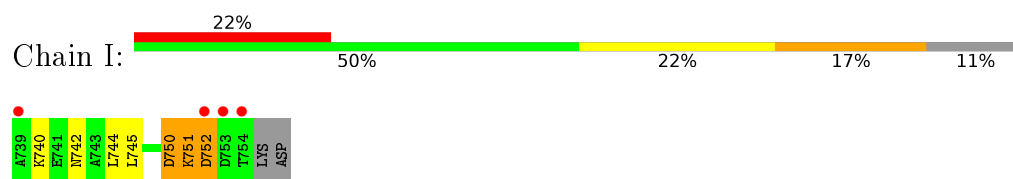
- Molecule 2: Orphan nuclear receptor NR1I3



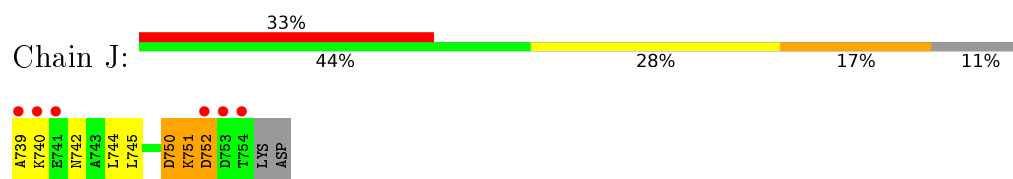
- Molecule 2: Orphan nuclear receptor NR1I3



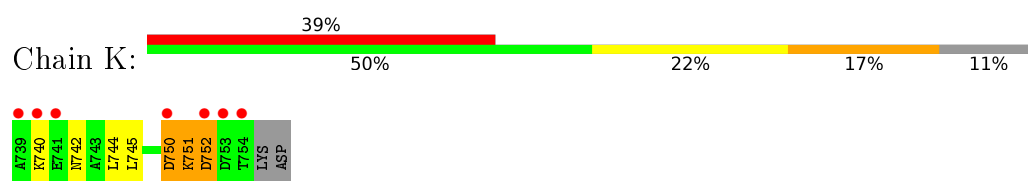
- Molecule 3: Nuclear receptor coactivator 2



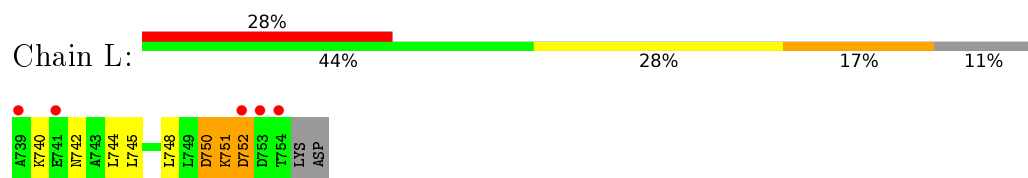
- Molecule 3: Nuclear receptor coactivator 2



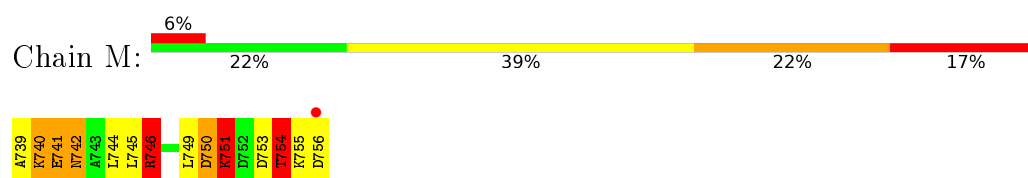
- Molecule 3: Nuclear receptor coactivator 2



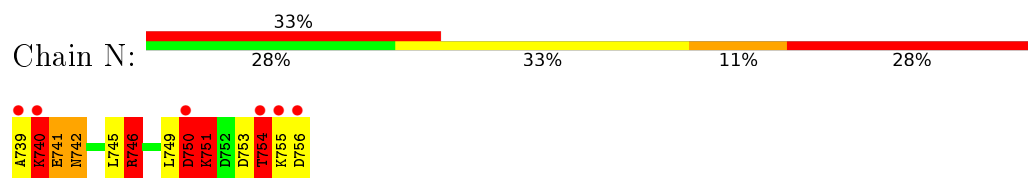
- Molecule 3: Nuclear receptor coactivator 2



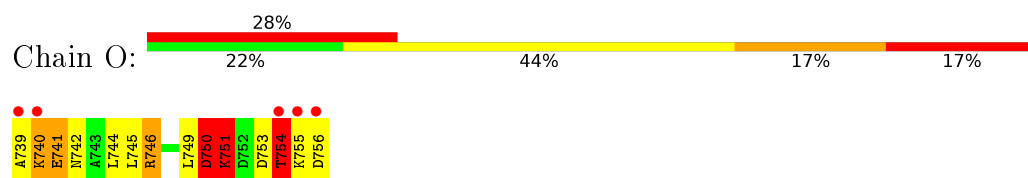
- Molecule 3: Nuclear receptor coactivator 2



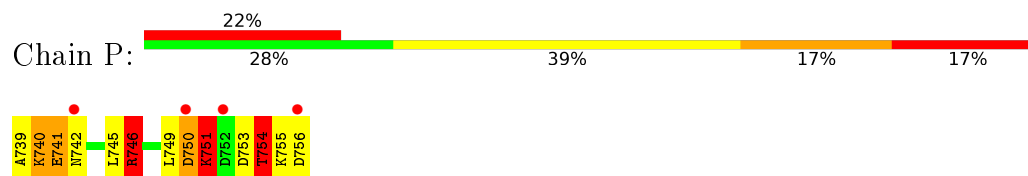
- Molecule 3: Nuclear receptor coactivator 2



- 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, $\alpha$ , $\beta$ , $\gamma$	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) 86.7 (19.99-2.97)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.98Å)	Xtrriage
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%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.2	Xtrriage
Anisotropy	0.008	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 57.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	16288	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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
1:C:284:LYS:HZ3	3:K:752:ASP:HB2	1.57	0.68
2:E:156:ARG:HB3	2:E:157:PRO:HA	1.75	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
1:B:284:LYS:HZ3	3:J:752:ASP:HB2	1.57	0.68
2:H:182:ILE:O	2:H:185:PHE:HB3	1.93	0.68
1:A:356:LYS:HG3	1:A:421:ARG:NH1	2.09	0.67
1:A:406:HIS:HE1	1:B:236:LEU:N	1.92	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:F:141:GLN:NE2	2:F:144:GLN:HE21	1.93	0.67
2:E:197:MET:HE1	3:M:749:LEU:HB2	1.76	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:197:MET:HE3	3:P:749:LEU:HD12	1.78	0.66
2:H:278:PHE:O	2:H:295:GLN:HB2	1.96	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
1:A:420:LEU:HA	2:E:323:MET:HE2	1.78	0.65
2:E:278:PHE:O	2:E:295:GLN:HB2	1.97	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:E:246:TYR:HH	2:G:246:TYR:HE1	1.48	0.62
2:G:168:LEU:HD13	2:G:349:MET:CE	2.30	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: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
1:C:420:LEU:HA	2:G:323:MET:CE	2.30	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
1:D:420:LEU:HA	2:H:323:MET:CE	2.30	0.61
2:E:187:LYS:HE2	3:M:749:LEU:HA	1.82	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
2:E:346:LEU:N	2:E:349:MET:HE2	2.15	0.60
2:E:175:ASN:HD22	2:E:353:LEU:HD11	1.67	0.60
1:B:284:LYS:HZ3	3:J:752:ASP:H	1.48	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:187:LYS:HE2	3:N:749:LEU:HA	1.83	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
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:275:GLN:HA	1:D:278:THR:HG23	1.86	0.58
1:D:232:VAL:HG23	1:D:399:SER:HB3	1.85	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:187:LYS:HE2	3:P:749:LEU:C	2.25	0.58
2:H:127:LEU:HB3	2:H:270:VAL:HG21	1.86	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
2:F:197:MET:HE3	3:N:749:LEU:CD1	2.35	0.56
1:D:420:LEU:HA	2:H:323:MET:HE2	1.86	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:196:THR:HG22	2:F:198:GLU:HG3	1.87	0.56
2:F:193:ARG:HA	2:F:200:GLN:OE1	2.05	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
1:D:397:TYR:HB3	2:H:317:PHE:CD1	2.42	0.54
2:E:158:PHE:HE2	2:E:241:HIS:HE2	1.51	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:240:VAL:CG2	2:H:241:HIS:N	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:168:LEU:HD22	2:H:346:LEU:HD13	1.90	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:168:LEU:HD13	2:F:349:MET:HE3	1.92	0.52
2:F:306:ILE:HD13	2:F:318:LEU:HD12	1.91	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:168:LEU:HD13	2:G:349:MET:HE3	1.93	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: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: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
2:G:187:LYS:HE2	3:O:749:LEU:CA	2.42	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
1:B:284:LYS:CD	3:J:752:ASP:HB2	2.43	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: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
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:D:284:LYS:HZ3	3:L:752:ASP:H	1.60	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
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
1:A:284:LYS:CD	3:I:752:ASP:HB2	2.43	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:F:168:LEU:HD22	2:F:346:LEU:HD13	1.96	0.47
2:E:160:PRO:HB2	2:G:164:VAL:HG11	1.95	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:139:PHE:CE2	2:E:216:LEU:HA	2.50	0.47
2:E:147:PRO:HB3	2:E:170:HIS:CE1	2.49	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:245:GLN:O	2:E:249:LEU:HD23	2.15	0.47
2:E:210:GLU:HG2	2:E:329:LEU:HB3	1.97	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
2:E:135:VAL:O	2:E:136:GLY:C	2.52	0.47
2:E:196:THR:HB	2:E:199:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:THR:HB	2:F:192:PHE:CD2	2.50	0.47
2:F:139:PHE:CE2	2:F:216:LEU:HA	2.50	0.47
1:B:419:LEU:HD13	2:F:320:ALA:HA	1.97	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:271:LEU:HB3	2:G:302:LEU:HD23	1.98	0.46
2:G:279:SER:HB2	2:G:282:ARG:HD2	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:209:VAL:HB	2:G:333:ASN:ND2	2.32	0.44
2:G:253:LEU:C	2:G:253:LEU:HD23	2.38	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
2:E:221:CYS:O	2:E:225:GLU:N	2.52	0.41
2:E:220:PHE:O	2:E:260:LYS:HE2	2.20	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
1:D:416:ALA:HB1	2:H:319:TYR:CZ	2.55	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:280:PRO:HB3	2:E:288:ARG:CG	2.50	0.41
2:E:201:ILE:HG23	3:M:745:LEU:HD13	2.02	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:273:ASP:OD1	1:B:449:THR:O	2.40	0.40
1:B:317:SER:OG	1:B:324:ILE:HA	2.22	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%)	2	10
1	B	230/232 (99%)	190 (83%)	27 (12%)	13 (6%)	2	10
1	C	230/232 (99%)	191 (83%)	25 (11%)	14 (6%)	2	9
1	D	230/232 (99%)	189 (82%)	27 (12%)	14 (6%)	2	9
2	E	240/242 (99%)	206 (86%)	22 (9%)	12 (5%)	3	13
2	F	240/242 (99%)	207 (86%)	20 (8%)	13 (5%)	2	11
2	G	240/242 (99%)	206 (86%)	21 (9%)	13 (5%)	2	11
2	H	240/242 (99%)	209 (87%)	18 (8%)	13 (5%)	2	11
3	I	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	6
3	J	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	6
3	K	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	6
3	L	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	6
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%)	2	9

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%)	9	30
1	B	182/200 (91%)	163 (90%)	19 (10%)	9	30
1	C	182/200 (91%)	163 (90%)	19 (10%)	9	30
1	D	182/200 (91%)	163 (90%)	19 (10%)	9	30
2	E	217/217 (100%)	191 (88%)	26 (12%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	217/217 (100%)	194 (89%)	23 (11%)	8	29
2	G	217/217 (100%)	193 (89%)	24 (11%)	8	27
2	H	217/217 (100%)	193 (89%)	24 (11%)	8	27
3	I	14/16 (88%)	10 (71%)	4 (29%)	0	2
3	J	14/16 (88%)	10 (71%)	4 (29%)	0	2
3	K	14/16 (88%)	10 (71%)	4 (29%)	0	2
3	L	14/16 (88%)	10 (71%)	4 (29%)	0	2
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%)	1	3
All	All	1716/1796 (96%)	1508 (88%)	208 (12%)	6	23

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	A	801	-	19,22,22	4.08	12 (63%)	26,30,30	2.92	15 (57%)
4	9CR	B	802	-	19,22,22	4.11	12 (63%)	26,30,30	2.93	15 (57%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	9CR	C	803	-	19,22,22	4.19	12 (63%)	26,30,30	2.95	15 (57%)
4	9CR	D	804	-	19,22,22	4.16	13 (68%)	26,30,30	2.92	14 (53%)
5	TCD	E	805	-	24,26,26	2.29	4 (16%)	24,36,36	1.63	6 (25%)
5	TCD	F	806	-	24,26,26	2.14	3 (12%)	24,36,36	1.39	3 (12%)
5	TCD	G	807	-	24,26,26	2.34	4 (16%)	24,36,36	1.58	5 (20%)
5	TCD	H	808	-	24,26,26	2.06	3 (12%)	24,36,36	1.45	4 (16%)

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

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	9CR	C4-C5	-4.61	1.41	1.51
4	D	804	9CR	C4-C5	-4.53	1.41	1.51
4	B	802	9CR	C4-C5	-4.50	1.41	1.51
4	C	803	9CR	C4-C5	-4.31	1.41	1.51
4	D	804	9CR	C3-C4	-3.59	1.40	1.52
4	A	801	9CR	C3-C4	-3.56	1.40	1.52
4	B	802	9CR	C3-C4	-3.47	1.40	1.52
4	C	803	9CR	C3-C4	-3.39	1.40	1.52
4	B	802	9CR	C8-C9	-2.87	1.39	1.45
4	C	803	9CR	C8-C9	-2.79	1.39	1.45
4	A	801	9CR	C8-C9	-2.71	1.39	1.45
4	D	804	9CR	C8-C9	-2.62	1.40	1.45
5	E	805	TCD	O31-C4	-2.14	1.34	1.39
4	D	804	9CR	C7-C8	2.03	1.39	1.32
5	G	807	TCD	C32-N33	2.20	1.37	1.32
5	E	805	TCD	C34-C35	2.32	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	801	9CR	C20-C13	2.35	1.55	1.50
5	G	807	TCD	C22-N23	2.37	1.37	1.32
5	G	807	TCD	C34-C35	2.37	1.42	1.38
4	B	802	9CR	C20-C13	2.44	1.55	1.50
4	C	803	9CR	C20-C13	2.55	1.55	1.50
4	D	804	9CR	C20-C13	2.56	1.55	1.50
4	A	801	9CR	C16-C1	2.72	1.59	1.53
4	B	802	9CR	C16-C1	2.73	1.59	1.53
4	C	803	9CR	C16-C1	2.74	1.59	1.53
4	D	804	9CR	C16-C1	2.91	1.60	1.53
5	H	808	TCD	C34-C35	2.96	1.43	1.38
5	E	805	TCD	C22-N23	3.00	1.39	1.32
4	B	802	9CR	C2-C3	3.00	1.60	1.52
4	A	801	9CR	C10-C9	3.01	1.39	1.35
4	D	804	9CR	C10-C9	3.01	1.39	1.35
4	A	801	9CR	C2-C3	3.09	1.60	1.52
4	C	803	9CR	C2-C3	3.13	1.60	1.52
4	D	804	9CR	C2-C3	3.16	1.60	1.52
5	H	808	TCD	C36-C35	3.21	1.43	1.38
5	F	806	TCD	C36-C35	3.27	1.43	1.38
4	B	802	9CR	C10-C9	3.32	1.40	1.35
4	C	803	9CR	C10-C9	3.58	1.40	1.35
4	A	801	9CR	C2-C1	3.58	1.62	1.54
4	B	802	9CR	C2-C1	3.59	1.62	1.54
5	F	806	TCD	C34-C35	3.61	1.45	1.38
4	D	804	9CR	C2-C1	3.65	1.62	1.54
4	C	803	9CR	C2-C1	3.71	1.63	1.54
4	C	803	9CR	C14-C13	4.33	1.41	1.35
4	D	804	9CR	C14-C13	4.33	1.41	1.35
4	A	801	9CR	C14-C13	4.39	1.41	1.35
4	B	802	9CR	C19-C9	4.52	1.59	1.50
4	B	802	9CR	C14-C13	4.52	1.41	1.35
4	C	803	9CR	C19-C9	4.55	1.59	1.50
4	A	801	9CR	C19-C9	4.70	1.59	1.50
4	D	804	9CR	C19-C9	4.71	1.59	1.50
5	H	808	TCD	C26-C27	7.59	1.51	1.38
5	F	806	TCD	C26-C27	7.83	1.51	1.38
4	B	802	9CR	C5-C6	9.06	1.50	1.34
4	A	801	9CR	C5-C6	9.06	1.50	1.34
4	D	804	9CR	C5-C6	9.12	1.50	1.34
5	E	805	TCD	C26-C27	9.27	1.54	1.38
4	C	803	9CR	C5-C6	9.43	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	807	TCD	C26-C27	9.49	1.54	1.38
4	A	801	9CR	C1-C6	9.75	1.67	1.53
4	B	802	9CR	C1-C6	9.96	1.67	1.53
4	D	804	9CR	C1-C6	10.21	1.67	1.53
4	C	803	9CR	C1-C6	10.25	1.68	1.53

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	801	9CR	C19-C9-C10	-5.76	114.52	122.89
4	D	804	9CR	C19-C9-C10	-5.75	114.52	122.89
4	C	803	9CR	C19-C9-C10	-5.73	114.56	122.89
4	B	802	9CR	C19-C9-C10	-5.73	114.56	122.89
4	B	802	9CR	C1-C6-C5	-5.56	115.06	122.50
4	C	803	9CR	C1-C6-C5	-5.53	115.10	122.50
4	D	804	9CR	C1-C6-C5	-5.51	115.13	122.50
4	A	801	9CR	C1-C6-C5	-5.47	115.18	122.50
4	D	804	9CR	C11-C10-C9	-3.58	122.02	127.22
4	A	801	9CR	C11-C10-C9	-3.52	122.11	127.22
4	B	802	9CR	C11-C10-C9	-3.40	122.28	127.22
4	C	803	9CR	C11-C10-C9	-3.32	122.39	127.22
4	B	802	9CR	C12-C13-C14	-2.54	112.26	119.00
4	A	801	9CR	C16-C1-C6	-2.51	106.50	110.33
4	B	802	9CR	C16-C1-C6	-2.50	106.51	110.33
4	C	803	9CR	C12-C13-C14	-2.49	112.39	119.00
4	A	801	9CR	C12-C13-C14	-2.48	112.41	119.00
4	D	804	9CR	C12-C13-C14	-2.48	112.42	119.00
4	C	803	9CR	C16-C1-C6	-2.45	106.59	110.33
4	D	804	9CR	C16-C1-C6	-2.32	106.79	110.33
4	C	803	9CR	C16-C1-C2	-2.17	101.12	108.75
4	B	802	9CR	C16-C1-C2	-2.16	101.16	108.75
4	D	804	9CR	C16-C1-C2	-2.16	101.17	108.75
5	E	805	TCD	C1-O21-C22	-2.16	114.32	118.85
5	H	808	TCD	C1-O21-C22	-2.13	114.38	118.85
4	A	801	9CR	C16-C1-C2	-2.07	101.47	108.75
4	A	801	9CR	C2-C1-C6	2.01	113.47	110.48
5	F	806	TCD	C27-C26-C25	2.03	120.92	118.72
4	D	804	9CR	C7-C6-C5	2.05	126.11	121.36
4	A	801	9CR	C7-C6-C5	2.05	126.12	121.36
4	A	801	9CR	C18-C5-C6	2.06	126.81	124.62
4	B	802	9CR	C7-C6-C5	2.08	126.18	121.36
5	G	807	TCD	C36-C35-CL35	2.09	121.91	119.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	804	9CR	C18-C5-C6	2.11	126.87	124.62
4	C	803	9CR	C7-C6-C5	2.13	126.31	121.36
4	C	803	9CR	C2-C1-C6	2.14	113.67	110.48
4	B	802	9CR	C2-C1-C6	2.19	113.74	110.48
5	H	808	TCD	C34-N33-C32	2.21	121.53	116.47
4	B	802	9CR	C18-C5-C6	2.28	127.05	124.62
5	E	805	TCD	C36-C35-CL35	2.37	122.28	119.13
4	C	803	9CR	C18-C5-C6	2.38	127.16	124.62
5	G	807	TCD	C4-O31-C32	2.42	123.93	118.85
5	E	805	TCD	C27-C26-C25	2.46	121.39	118.72
5	G	807	TCD	C27-C26-C25	2.51	121.44	118.72
5	E	805	TCD	C24-N23-C22	2.62	122.47	116.47
5	F	806	TCD	C36-C35-CL35	2.63	122.63	119.13
5	F	806	TCD	C24-N23-C22	2.67	122.58	116.47
5	E	805	TCD	C4-O31-C32	2.71	124.54	118.85
5	H	808	TCD	C24-N23-C22	2.71	122.67	116.47
5	G	807	TCD	C24-N23-C22	2.71	122.68	116.47
4	B	802	9CR	C8-C7-C6	2.76	135.24	127.24
5	H	808	TCD	C36-C35-CL35	2.79	122.84	119.13
4	C	803	9CR	C8-C7-C6	2.80	135.38	127.24
4	A	801	9CR	C8-C7-C6	2.83	135.47	127.24
4	D	804	9CR	C8-C7-C6	2.86	135.54	127.24
5	E	805	TCD	C37-C36-C35	3.05	122.03	118.72
5	G	807	TCD	C37-C36-C35	3.51	122.53	118.72
4	A	801	9CR	C20-C13-C12	4.03	124.67	118.08
4	B	802	9CR	C19-C9-C8	4.06	124.71	118.08
4	C	803	9CR	C19-C9-C8	4.06	124.72	118.08
4	D	804	9CR	C20-C13-C12	4.07	124.74	118.08
4	A	801	9CR	C19-C9-C8	4.12	124.82	118.08
4	D	804	9CR	C19-C9-C8	4.15	124.86	118.08
4	B	802	9CR	C20-C13-C12	4.17	124.89	118.08
4	C	803	9CR	C20-C13-C12	4.22	124.98	118.08
4	B	802	9CR	C7-C8-C9	4.46	132.95	126.21
4	A	801	9CR	C7-C8-C9	4.48	132.97	126.21
4	A	801	9CR	C3-C4-C5	4.49	121.31	113.87
4	D	804	9CR	C7-C8-C9	4.53	133.05	126.21
4	C	803	9CR	C7-C8-C9	4.55	133.09	126.21
4	D	804	9CR	C3-C4-C5	4.59	121.48	113.87
4	B	802	9CR	C3-C4-C5	4.60	121.48	113.87
4	C	803	9CR	C3-C4-C5	4.72	121.70	113.87
4	D	804	9CR	C17-C1-C6	4.87	117.78	110.33
4	B	802	9CR	C17-C1-C6	4.92	117.85	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	803	9CR	C17-C1-C6	4.97	117.92	110.33
4	A	801	9CR	C17-C1-C6	5.08	118.09	110.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	232/232 (100%)	0.42	24 (10%) 9 4	22, 47, 126, 134	0
1	B	232/232 (100%)	0.54	25 (10%) 8 4	22, 50, 128, 137	0
1	C	232/232 (100%)	0.56	26 (11%) 7 4	21, 53, 127, 136	0
1	D	232/232 (100%)	0.43	21 (9%) 11 6	21, 50, 125, 135	0
2	E	242/242 (100%)	-0.04	12 (4%) 32 19	21, 44, 89, 122	0
2	F	242/242 (100%)	0.10	14 (5%) 26 14	16, 42, 89, 127	0
2	G	242/242 (100%)	0.15	19 (7%) 15 8	17, 44, 88, 126	0
2	H	242/242 (100%)	-0.01	15 (6%) 24 13	18, 44, 89, 121	0
3	I	16/18 (88%)	1.36	4 (25%) 1 1	43, 79, 130, 135	0
3	J	16/18 (88%)	2.41	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%)	1.25	5 (31%) 1 0	43, 77, 131, 137	0
3	M	18/18 (100%)	0.96	1 (5%) 28 15	37, 77, 121, 125	0
3	N	18/18 (100%)	1.66	6 (33%) 0 0	39, 76, 121, 129	0
3	O	18/18 (100%)	1.40	5 (27%) 1 0	39, 75, 120, 129	0
3	P	18/18 (100%)	0.94	4 (22%) 1 1	37, 80, 120, 124	0
All	All	2032/2040 (99%)	0.35	194 (9%) 10 5	16, 48, 120, 137	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	249	TYR	14.3
1	B	248	THR	14.0
1	C	255	GLY	12.3
3	K	754	THR	11.2
1	D	254	MET	10.7

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Mol	Chain	Res	Type	RSRZ
2	G	161	ARG	10.3
1	D	251	GLU	10.3
1	D	252	ALA	10.1
1	B	249	TYR	9.8
1	A	250	VAL	9.5
3	J	753	ASP	9.4
3	O	739	ALA	9.4
1	D	248	THR	9.0
1	B	255	GLY	9.0
1	C	248	THR	9.0
1	D	260	SER	8.9
1	C	457	ALA	8.8
1	B	253	ASN	8.7
1	C	254	MET	8.7
3	J	754	THR	8.7
1	B	254	MET	8.5
1	C	256	LEU	8.4
1	D	249	TYR	8.2
1	C	458	PRO	8.1
3	K	753	ASP	8.1
1	B	256	LEU	8.0
2	F	161	ARG	7.9
3	J	752	ASP	7.8
1	B	247	GLU	7.7
1	C	257	ASN	7.6
1	A	253	ASN	7.5
1	D	247	GLU	7.4
1	D	253	ASN	7.3
1	B	458	PRO	7.3
2	F	162	GLY	7.1
1	A	252	ALA	7.1
3	N	739	ALA	7.1
1	B	246	THR	7.1
1	B	262	ASN	7.0
2	G	162	GLY	6.9
3	L	739	ALA	6.8
2	F	160	PRO	6.7
1	A	257	ASN	6.6
3	I	739	ALA	6.6
3	K	752	ASP	6.5
1	C	260	SER	6.5
3	L	754	THR	6.3

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Mol	Chain	Res	Type	RSRZ
3	J	739	ALA	6.1
1	C	247	GLU	6.0
1	B	252	ALA	5.9
1	B	257	ASN	5.8
1	A	260	SER	5.7
2	G	157	PRO	5.6
1	B	261	PRO	5.5
1	A	258	PRO	5.4
2	F	159	GLN	5.4
1	D	250	VAL	5.4
2	G	154	HIS	5.4
2	G	159	GLN	5.3
3	N	740	LYS	5.2
1	A	244	PRO	5.2
1	C	262	ASN	5.2
1	C	251	GLU	5.2
1	A	254	MET	5.1
1	A	458	PRO	5.0
3	P	756	ASP	5.0
2	G	160	PRO	5.0
1	A	251	GLU	5.0
1	D	257	ASN	4.8
1	C	252	ALA	4.8
3	I	754	THR	4.8
1	B	245	LYS	4.8
1	B	260	SER	4.8
2	H	310	GLN	4.8
2	F	157	PRO	4.7
2	G	312	ARG	4.7
1	C	261	PRO	4.6
3	O	756	ASP	4.6
3	N	756	ASP	4.6
2	E	312	ARG	4.5
3	I	753	ASP	4.5
3	M	756	ASP	4.5
3	K	739	ALA	4.4
2	G	313	LEU	4.4
1	C	444	ASP	4.4
3	L	741	GLU	4.3
1	A	245	LYS	4.3
1	D	246	THR	4.2
1	B	250	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
2	E	310	GLN	4.2
2	G	342	ARG	4.2
2	F	312	ARG	4.1
1	B	457	ALA	4.1
1	D	335	ASN	4.1
2	H	161	ARG	4.0
1	B	243	GLU	4.0
1	C	253	ASN	4.0
1	C	249	TYR	4.0
1	C	229	ASP	4.0
2	H	160	PRO	4.0
1	B	251	GLU	3.9
3	P	742	ASN	3.9
2	E	342	ARG	3.8
2	E	358	SER	3.7
1	D	458	PRO	3.7
1	C	227	ASN	3.6
3	O	754	THR	3.6
1	C	246	THR	3.6
1	D	227	ASN	3.6
1	A	248	THR	3.5
1	B	227	ASN	3.5
2	F	311	SER	3.4
2	G	314	GLN	3.4
2	G	158	PHE	3.4
3	N	755	LYS	3.4
2	F	154	HIS	3.4
2	F	163	PRO	3.3
1	C	245	LYS	3.2
1	D	258	PRO	3.2
2	H	312	ARG	3.2
1	A	255	GLY	3.2
2	G	163	PRO	3.2
2	E	160	PRO	3.1
2	G	310	GLN	3.1
2	G	311	SER	3.1
2	H	155	HIS	3.1
2	H	311	SER	3.0
2	E	316	ARG	3.0
2	H	342	ARG	3.0
1	C	442	ILE	2.9
1	D	322	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	133	ARG	2.9
3	L	753	ASP	2.9
1	D	244	PRO	2.9
1	A	338	HIS	2.8
3	N	750	ASP	2.8
2	H	316	ARG	2.8
2	E	158	PHE	2.7
2	H	358	SER	2.7
3	I	752	ASP	2.7
1	A	261	PRO	2.7
1	A	243	GLU	2.6
3	K	740	LYS	2.6
2	F	158	PHE	2.6
1	C	242	VAL	2.6
1	A	227	ASN	2.6
2	E	311	SER	2.5
3	J	741	GLU	2.5
3	N	754	THR	2.5
2	F	156	ARG	2.5
2	G	316	ARG	2.5
1	B	258	PRO	2.5
2	E	161	ARG	2.5
1	C	250	VAL	2.5
1	C	456	GLU	2.5
1	D	255	GLY	2.5
3	O	755	LYS	2.5
3	O	740	LYS	2.4
1	A	334	ARG	2.4
1	B	228	GLU	2.4
1	A	369	CYS	2.3
2	H	117	ASN	2.3
2	E	155	HIS	2.3
1	A	246	THR	2.3
1	D	240	LEU	2.3
2	H	118	GLN	2.3
1	A	247	GLU	2.3
2	G	155	HIS	2.3
2	E	157	PRO	2.3
2	F	313	LEU	2.3
2	G	156	ARG	2.2
1	D	261	PRO	2.2
3	K	741	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	256	LEU	2.2
1	C	322	ASP	2.2
2	H	236	MET	2.2
1	D	406	HIS	2.2
2	G	247	GLU	2.2
2	F	316	ARG	2.2
2	G	198	GLU	2.2
1	B	244	PRO	2.1
2	H	132	THR	2.1
1	A	259	SER	2.1
2	H	158	PHE	2.1
3	L	752	ASP	2.1
1	B	340	ALA	2.1
3	P	750	ASP	2.1
3	J	740	LYS	2.1
1	B	268	ILE	2.0
3	K	750	ASP	2.0
2	F	133	ARG	2.0
1	C	359	ASP	2.0
3	P	752	ASP	2.0
2	E	122	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	TCD	E	805	24/24	0.81	0.30	4.96	27,42,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	9CR	A	801	22/22	0.92	0.39	3.53	31,43,48,53	0
4	9CR	D	804	22/22	0.93	0.33	3.09	31,39,44,49	0
5	TCD	H	808	24/24	0.82	0.27	3.03	27,37,54,54	0
4	9CR	C	803	22/22	0.86	0.26	1.36	32,41,48,48	0
4	9CR	B	802	22/22	0.90	0.27	1.18	26,36,41,47	0
5	TCD	G	807	24/24	0.89	0.22	0.92	12,38,54,54	0
5	TCD	F	806	24/24	0.92	0.19	0.28	14,35,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.