



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:26 pm BST

PDB ID : 2ACL  
Title : Liver X-Receptor alpha Ligand Binding Domain with SB313987  
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Deposited on : 2005-07-19  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

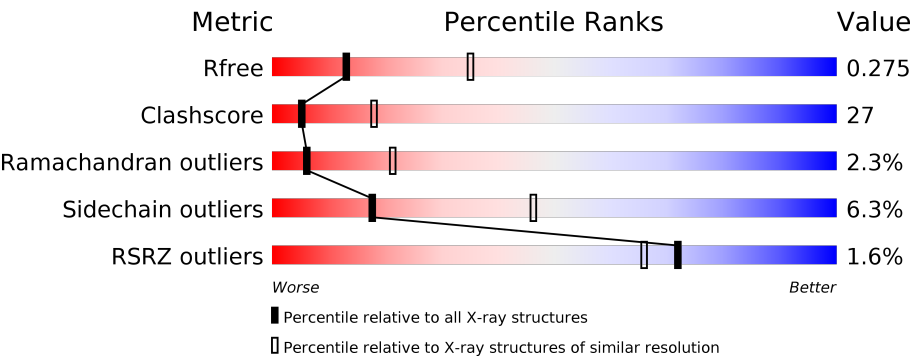
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	238	<div><div>%</div><div><div></div><div>50%</div><div>35%</div><div>5%</div><div>10%</div></div></div>
1	C	238	<div><div></div><div>56%</div><div>32%</div><div>•</div><div>10%</div></div>
1	E	238	<div><div></div><div>55%</div><div>31%</div><div>5%</div><div>10%</div></div>
1	G	238	<div><div>%</div><div><div></div><div>47%</div><div>39%</div><div>•</div><div>10%</div></div></div>
2	B	244	<div><div>2%</div><div><div></div><div>52%</div><div>42%</div><div>5%</div><div>••</div></div></div>
2	D	244	<div><div></div><div>51%</div><div>44%</div><div>••</div></div>

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Mol	Chain	Length	Quality of chain
2	F	244	<div><div></div><div>4%</div><div>55%</div><div>39%</div><div>5%</div><div></div></div>
2	H	244	<div><div></div><div>4%</div><div>45%</div><div>52%</div><div></div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14858 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	214	Total	C	N	O	S	0	0	0
			1682	1078	289	305	10			
1	C	215	Total	C	N	O	S	0	0	0
			1689	1083	290	306	10			
1	E	214	Total	C	N	O	S	0	0	0
			1682	1078	289	305	10			
1	G	214	Total	C	N	O	S	0	0	0
			1682	1078	289	305	10			

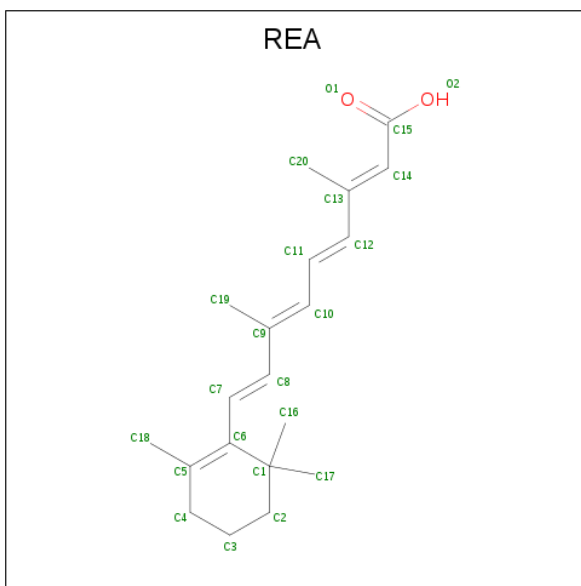
- Molecule 2 is a protein called Oxysterols receptor LXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	242	Total	C	N	O	S	0	0	0
			1966	1255	343	361	7			
2	D	242	Total	C	N	O	S	0	0	0
			1966	1255	343	361	7			
2	F	242	Total	C	N	O	S	0	0	0
			1966	1255	343	361	7			
2	H	244	Total	C	N	O	S	0	0	0
			1985	1266	347	365	7			

There are 8 discrepancies between the modelled and reference sequences:

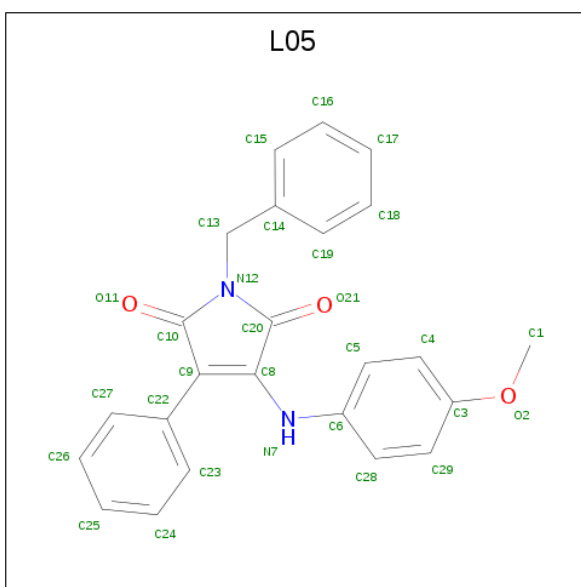
Chain	Residue	Modelled	Actual	Comment	Reference
B	202	VAL	-	CLONING ARTIFACT	UNP Q9Z0Y9
B	399	PRO	ARG	VARIANT	UNP Q9Z0Y9
D	202	VAL	-	CLONING ARTIFACT	UNP Q9Z0Y9
D	399	PRO	ARG	VARIANT	UNP Q9Z0Y9
F	202	VAL	-	CLONING ARTIFACT	UNP Q9Z0Y9
F	399	PRO	ARG	VARIANT	UNP Q9Z0Y9
H	202	VAL	-	CLONING ARTIFACT	UNP Q9Z0Y9
H	399	PRO	ARG	VARIANT	UNP Q9Z0Y9

- Molecule 3 is RETINOIC ACID (three-letter code: REA) (formula:  $C_{20}H_{28}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	20	2		
3	C	1	Total	C	O	0	0
			22	20	2		
3	E	1	Total	C	O	0	0
			22	20	2		
3	G	1	Total	C	O	0	0
			22	20	2		

- Molecule 4 is 1-BENZYL-3-(4-METHOXYPHENYLAMINO)-4-PHENYLPYRROLE-2,5-DIONE (three-letter code: L05) (formula:  $C_{24}H_{20}N_2O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			29	24	2	3		
4	D	1	Total	C	N	O	0	0
			29	24	2	3		
4	F	1	Total	C	N	O	0	0
			29	24	2	3		
4	H	1	Total	C	N	O	0	0
			29	24	2	3		

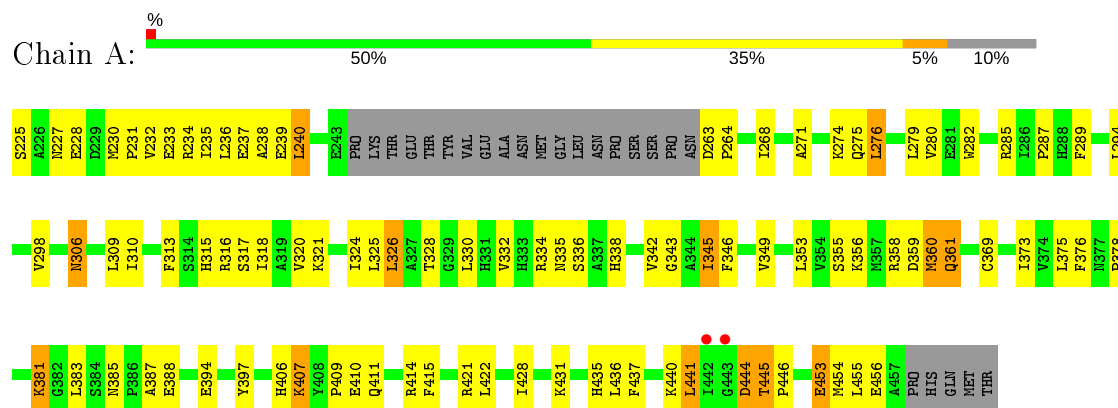
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	4	Total	O	0	0
			4	4		
5	C	3	Total	O	0	0
			3	3		
5	D	7	Total	O	0	0
			7	7		
5	E	4	Total	O	0	0
			4	4		
5	F	6	Total	O	0	0
			6	6		
5	G	5	Total	O	0	0
			5	5		
5	H	2	Total	O	0	0
			2	2		

### 3 Residue-property plots

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

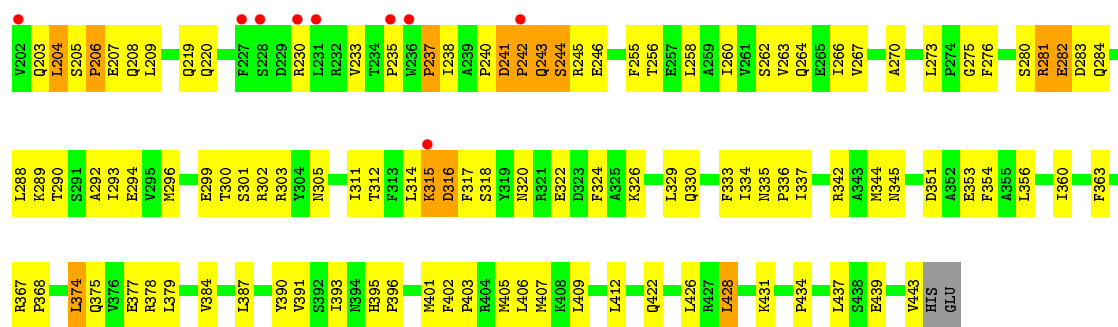
#### • Molecule 1: Retinoic acid receptor RXR-alpha






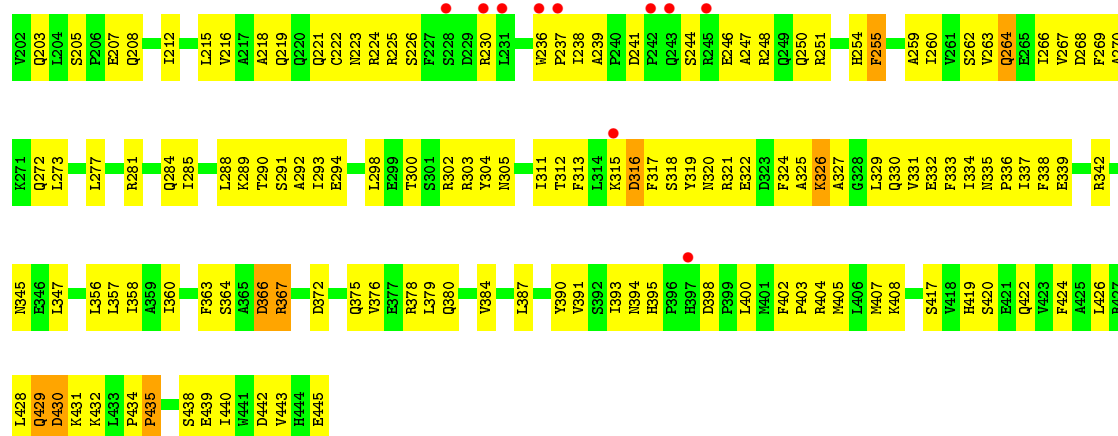


Chain F: 



• Molecule 2: Oxysterols receptor LXR-alpha

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.77Å 81.95Å 111.44Å 88.98° 75.20° 78.27°	Depositor
Resolution (Å)	30.00 – 2.80 45.58 – 2.74	Depositor EDS
% Data completeness (in resolution range)	95.0 (30.00-2.80) 89.3 (45.58-2.74)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.73Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.210 , 0.280 0.205 , 0.275	Depositor DCC
$R_{free}$ test set	2415 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,-h+l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14858	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: L05, REA

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	0.39	0/1714	0.64	0/2317
1	C	0.42	0/1722	0.63	0/2329
1	E	0.37	0/1714	0.62	0/2317
1	G	0.40	0/1714	0.61	0/2317
2	B	0.40	0/2008	0.60	0/2721
2	D	0.42	0/2008	0.59	0/2721
2	F	0.38	0/2008	0.54	0/2721
2	H	0.39	0/2028	0.56	0/2748
All	All	0.39	0/14916	0.60	0/20191

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1682	0	1713	101	0
1	C	1689	0	1720	82	0
1	E	1682	0	1713	80	0
1	G	1682	0	1713	115	0
2	B	1966	0	1973	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1966	0	1973	129	0
2	F	1966	0	1973	94	0
2	H	1985	0	1986	154	0
3	A	22	0	27	0	0
3	C	22	0	27	0	0
3	E	22	0	27	0	0
3	G	22	0	27	0	0
4	B	29	0	20	0	0
4	D	29	0	20	2	0
4	F	29	0	20	1	0
4	H	29	0	20	1	0
5	A	5	0	0	0	0
5	B	4	0	0	1	0
5	C	3	0	0	1	0
5	D	7	0	0	0	0
5	E	4	0	0	0	0
5	F	6	0	0	2	0
5	G	5	0	0	0	0
5	H	2	0	0	2	0
All	All	14858	0	14952	793	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (793) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:HD22	1:A:388:GLU:HG3	1.31	0.95
2:H:387:LEU:O	2:H:391:VAL:HG22	1.69	0.91
1:E:454:MET:HE2	2:F:263:VAL:HG12	1.52	0.91
2:F:299:GLU:HG3	2:F:303:ARG:HH12	1.33	0.91
1:C:302:ARG:HH12	2:H:330:GLN:HE22	1.22	0.88
1:G:227:ASN:HD21	1:G:232:VAL:HG22	1.36	0.87
1:G:236:LEU:HD22	1:G:240:LEU:HD22	1.57	0.87
2:B:378:ARG:HB3	2:B:378:ARG:HH11	1.39	0.86
2:H:225:ARG:HH21	2:H:268:ASP:HB3	1.41	0.86
2:F:305:ASN:HD21	2:F:312:THR:HG23	1.37	0.85
1:G:380:SER:HB2	1:G:383:LEU:HD21	1.58	0.85
1:G:334:ARG:HD2	1:G:347:ASP:OD1	1.76	0.85
2:H:241:ASP:HB3	2:H:244:SER:HB2	1.59	0.84
1:A:385:ASN:ND2	1:A:388:GLU:HG3	1.91	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:HD3	1:A:275:GLN:HE21	1.43	0.84
2:F:299:GLU:HG3	2:F:303:ARG:NH1	1.91	0.83
2:H:238:ILE:HG13	2:H:239:ALA:H	1.42	0.83
1:G:421:ARG:HA	1:G:421:ARG:HE	1.41	0.83
1:C:227:ASN:ND2	1:C:232:VAL:HG22	1.93	0.83
2:F:230:ARG:HG2	2:F:314:LEU:HD13	1.59	0.82
2:D:243:GLN:HE21	1:G:294:LEU:H	1.27	0.82
1:A:446:PRO:HB3	2:B:443:VAL:HB	1.60	0.82
2:D:219:GLN:NE2	2:D:302:ARG:HH22	1.77	0.82
1:A:385:ASN:HD21	1:A:387:ALA:HB3	1.44	0.82
1:C:230:MET:HE3	1:C:235:ILE:HD11	1.62	0.81
2:H:241:ASP:CB	2:H:244:SER:HB2	2.11	0.81
1:A:356:LYS:HG3	1:A:421:ARG:NH1	1.96	0.81
2:F:374:LEU:HD12	2:F:378:ARG:NH1	1.96	0.80
2:D:243:GLN:NE2	1:G:294:LEU:H	1.78	0.80
1:A:355:SER:HA	1:A:358:ARG:NH1	1.96	0.80
1:E:307:GLU:HG2	1:E:425:LEU:HG	1.62	0.80
1:G:394:GLU:HA	1:G:397:TYR:CD2	2.16	0.80
2:F:294:GLU:HG2	2:F:412:LEU:HB3	1.62	0.80
2:H:375:GLN:HA	2:H:378:ARG:HE	1.45	0.80
2:D:229:ASP:O	2:D:232:ARG:HG2	1.82	0.80
1:G:325:LEU:HD13	1:G:331:HIS:CE1	2.18	0.79
1:A:230:MET:CE	1:A:235:ILE:HD11	2.12	0.79
2:B:248:ARG:HH12	2:B:431:LYS:HE2	1.47	0.79
1:G:421:ARG:NE	1:G:421:ARG:HA	1.96	0.79
1:A:233:GLU:O	1:A:237:GLU:HG3	1.83	0.79
2:H:315:LYS:O	2:H:316:ASP:HB2	1.82	0.79
1:E:306:ASN:H	1:E:306:ASN:HD22	1.31	0.79
1:G:441:LEU:HB2	2:H:445:GLU:OE1	1.81	0.79
2:F:204:LEU:H	2:F:393:ILE:HD11	1.48	0.78
1:C:269:CYS:HB3	2:H:445:GLU:OE2	1.84	0.78
2:H:375:GLN:HB2	2:H:378:ARG:HH21	1.48	0.78
2:H:380:GLN:O	2:H:384:VAL:HG23	1.84	0.78
2:F:219:GLN:NE2	2:F:302:ARG:HH22	1.82	0.77
1:C:347:ASP:O	1:C:351:THR:HG23	1.85	0.77
2:H:320:ASN:HD21	2:H:322:GLU:HB3	1.49	0.77
2:B:300:THR:HG22	2:B:311:ILE:HD13	1.67	0.77
1:C:357:MET:HG2	1:C:362:MET:HE3	1.64	0.77
1:E:410:GLU:O	1:E:412:PRO:HD3	1.84	0.77
1:A:397:TYR:OH	2:B:407:MET:HG3	1.84	0.77
2:H:262:SER:O	2:H:266:ILE:HG13	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ASN:HD21	1:E:232:VAL:HG22	1.49	0.77
2:B:430:ASP:HB2	1:E:280:VAL:HG11	1.66	0.76
2:D:342:ARG:HB3	2:D:342:ARG:NH1	2.01	0.76
2:H:387:LEU:HD21	2:H:405:MET:HE2	1.65	0.76
1:A:394:GLU:HA	1:A:397:TYR:CD2	2.20	0.76
1:E:321:LYS:HE3	1:E:322:ASP:OD2	1.85	0.76
1:C:227:ASN:HD21	1:C:232:VAL:H	1.34	0.75
2:H:400:LEU:O	2:H:403:PRO:HD2	1.86	0.75
2:D:330:GLN:N	2:D:330:GLN:HE21	1.84	0.75
1:C:304:GLY:HA2	5:C:23:HOH:O	1.86	0.75
1:C:356:LYS:O	1:C:360:MET:HG2	1.86	0.75
2:D:437:LEU:O	2:D:440:ILE:HD13	1.87	0.75
2:H:356:LEU:HD13	2:H:387:LEU:HA	1.67	0.75
2:H:429:GLN:O	2:H:430:ASP:HB3	1.87	0.75
2:F:387:LEU:O	2:F:391:VAL:HG22	1.88	0.74
2:F:434:PRO:HD2	2:F:437:LEU:HD12	1.70	0.74
1:G:347:ASP:O	1:G:351:THR:HG23	1.86	0.73
2:B:243:GLN:HG3	2:B:248:ARG:HD2	1.70	0.73
2:F:256:THR:O	2:F:260:ILE:HG12	1.88	0.73
1:A:227:ASN:HD21	1:A:232:VAL:HG22	1.52	0.73
1:C:227:ASN:HD21	1:C:232:VAL:HG22	1.54	0.73
2:B:227:PHE:CE1	2:B:315:LYS:HG3	2.24	0.72
2:D:428:LEU:H	2:D:428:LEU:HD22	1.55	0.72
1:G:356:LYS:HG3	1:G:421:ARG:NH1	2.04	0.72
2:H:305:ASN:HD21	2:H:312:THR:HG23	1.53	0.72
2:F:280:SER:OG	2:F:282:GLU:HG2	1.89	0.71
2:B:330:GLN:HG3	2:B:332:GLU:HG2	1.72	0.71
1:C:357:MET:HG2	1:C:362:MET:CE	2.20	0.71
1:C:236:LEU:HD22	1:C:240:LEU:HD22	1.69	0.71
2:B:400:LEU:O	2:B:403:PRO:HD2	1.90	0.71
2:B:300:THR:CG2	2:B:311:ILE:HD13	2.21	0.71
2:B:402:PHE:HB3	2:B:403:PRO:HD3	1.73	0.71
2:D:260:ILE:HG23	2:D:436:LEU:HD23	1.71	0.71
1:C:230:MET:CE	1:C:235:ILE:HD11	2.21	0.71
1:C:390:GLU:O	1:C:394:GLU:HG3	1.90	0.71
1:E:230:MET:CE	1:E:235:ILE:HD11	2.21	0.71
1:E:282:TRP:CZ3	1:E:375:LEU:HD22	2.25	0.71
2:D:219:GLN:HE22	2:D:302:ARG:HH22	1.38	0.70
2:F:387:LEU:HD21	2:F:405:MET:HE3	1.73	0.70
2:H:364:SER:HB2	2:H:367:ARG:HH11	1.57	0.70
1:A:385:ASN:ND2	1:A:387:ALA:HB3	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:333:PHE:CE2	2:D:337:ILE:HD11	2.27	0.69
1:G:353:LEU:O	1:G:357:MET:HG3	1.93	0.69
1:A:421:ARG:HA	1:A:421:ARG:NE	2.06	0.69
1:G:334:ARG:HD3	1:G:350:LEU:HD12	1.75	0.69
1:A:349:VAL:HG13	1:A:353:LEU:HD12	1.73	0.69
1:C:422:LEU:HD12	2:D:407:MET:CE	2.23	0.69
1:C:454:MET:HE1	2:D:264:GLN:HB2	1.74	0.69
2:F:374:LEU:HD12	2:F:378:ARG:HH12	1.57	0.69
1:C:422:LEU:HD12	2:D:407:MET:HE3	1.73	0.69
2:B:254:HIS:HE2	2:B:319:TYR:HH	1.40	0.69
1:A:415:PHE:HE2	2:B:403:PRO:HG3	1.57	0.69
2:D:330:GLN:CA	2:D:330:GLN:HE21	2.06	0.68
2:H:364:SER:CB	2:H:367:ARG:HH11	2.06	0.68
1:G:392:LEU:O	1:G:396:VAL:HG23	1.94	0.68
1:C:443:GLY:HA3	2:D:443:VAL:HG11	1.76	0.68
2:D:241:ASP:H	2:D:242:PRO:HD3	1.58	0.67
1:E:236:LEU:HD22	1:E:240:LEU:CD2	2.24	0.67
1:E:334:ARG:NH1	1:E:347:ASP:OD1	2.28	0.67
1:C:227:ASN:ND2	1:C:232:VAL:H	1.91	0.67
1:C:440:LYS:HG3	1:G:266:THR:HG23	1.76	0.67
1:G:381:LYS:N	1:G:381:LYS:HD2	2.10	0.66
1:A:230:MET:HE2	1:A:235:ILE:HD11	1.76	0.66
1:C:443:GLY:HA3	2:D:443:VAL:CG1	2.25	0.66
1:G:315:HIS:CG	1:G:367:LEU:HD22	2.30	0.66
2:B:237:PRO:HG3	2:B:250:GLN:HB3	1.77	0.66
2:B:287:LEU:O	2:B:291:SER:HB3	1.95	0.66
2:H:342:ARG:O	2:H:345:ASN:HB3	1.95	0.66
1:G:446:PRO:O	1:G:447:ILE:HG13	1.96	0.66
1:A:355:SER:HA	1:A:358:ARG:HH12	1.59	0.66
2:D:254:HIS:NE2	2:D:319:TYR:OH	2.27	0.66
2:F:428:LEU:HD22	2:F:428:LEU:H	1.61	0.66
1:G:334:ARG:HD3	1:G:350:LEU:CD1	2.26	0.65
2:B:231:LEU:O	2:B:231:LEU:HD23	1.96	0.65
2:F:230:ARG:CG	2:F:314:LEU:HD13	2.27	0.65
1:G:380:SER:HB2	1:G:383:LEU:CD2	2.26	0.65
2:B:203:GLN:HG2	2:B:204:LEU:H	1.61	0.65
1:C:230:MET:CE	1:C:396:VAL:HG22	2.26	0.65
1:G:356:LYS:HG3	1:G:421:ARG:HH11	1.59	0.65
2:D:350:ASN:OD1	2:D:353:GLU:HG3	1.97	0.65
2:F:312:THR:HG22	2:F:318:SER:HB2	1.79	0.65
1:A:385:ASN:ND2	1:A:388:GLU:H	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ALA:CB	1:A:326:LEU:HD12	2.27	0.65
1:G:316:ARG:HG2	1:G:316:ARG:HH11	1.61	0.65
1:A:349:VAL:O	1:A:353:LEU:HB2	1.97	0.64
2:B:248:ARG:NE	1:E:294:LEU:HD23	2.12	0.64
2:B:335:ASN:HB2	2:B:336:PRO:HD3	1.79	0.64
2:F:387:LEU:HD11	2:F:405:MET:HE1	1.79	0.64
1:G:236:LEU:HD22	1:G:240:LEU:CD2	2.26	0.64
2:H:289:LYS:NZ	2:H:440:ILE:HA	2.11	0.64
2:B:204:LEU:HD12	2:B:208:GLN:OE1	1.97	0.64
2:F:322:GLU:HG2	2:F:326:LYS:HE3	1.79	0.64
2:H:330:GLN:OE1	2:H:422:GLN:HB2	1.96	0.64
1:G:230:MET:CE	1:G:235:ILE:HD11	2.27	0.64
2:H:237:PRO:HB2	2:H:251:ARG:NH1	2.12	0.64
1:G:264:PRO:HG2	1:G:336:SER:HB3	1.80	0.64
2:H:303:ARG:HD3	2:H:312:THR:O	1.98	0.64
2:F:303:ARG:HD3	2:F:312:THR:O	1.98	0.63
2:D:219:GLN:HE22	2:D:302:ARG:NH2	1.96	0.63
1:G:380:SER:O	1:G:383:LEU:HD23	1.98	0.63
1:G:348:ARG:O	1:G:352:GLU:HB2	1.99	0.63
2:D:364:SER:O	2:D:367:ARG:HG2	1.99	0.63
1:E:318:ILE:HG23	1:E:358:ARG:HG3	1.80	0.63
2:F:333:PHE:CE2	2:F:337:ILE:HD11	2.34	0.63
2:F:204:LEU:N	2:F:393:ILE:HD11	2.13	0.63
2:D:330:GLN:O	2:D:334:ILE:HG13	1.98	0.62
2:H:400:LEU:CB	2:H:404:ARG:HH21	2.12	0.62
1:C:334:ARG:HD2	1:C:347:ASP:OD1	1.98	0.62
2:D:428:LEU:HD11	1:G:276:LEU:HD21	1.81	0.62
1:E:397:TYR:OH	2:F:407:MET:HG3	2.00	0.62
1:C:302:ARG:HH22	2:H:330:GLN:HE21	1.47	0.62
1:G:422:LEU:HD12	2:H:407:MET:HE3	1.81	0.62
2:H:400:LEU:HB2	2:H:404:ARG:HH21	1.65	0.62
2:B:238:ILE:HD12	2:B:238:ILE:H	1.64	0.62
2:B:320:ASN:ND2	2:B:323:ASP:H	1.97	0.62
1:C:333:HIS:HD2	1:C:334:ARG:N	1.97	0.62
2:F:238:ILE:O	2:F:240:PRO:HD3	1.99	0.62
1:E:422:LEU:HD12	2:F:407:MET:HE3	1.82	0.62
2:H:402:PHE:HB3	2:H:403:PRO:HD3	1.82	0.62
2:B:238:ILE:HD12	2:B:238:ILE:N	2.14	0.62
2:D:237:PRO:HG2	2:D:250:GLN:CB	2.30	0.61
2:H:225:ARG:NH2	2:H:268:ASP:HB3	2.15	0.61
1:C:302:ARG:HH12	2:H:330:GLN:NE2	1.95	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:235:PRO:O	2:D:237:PRO:HD3	1.99	0.61
2:F:219:GLN:NE2	2:F:302:ARG:NH2	2.47	0.61
2:B:254:HIS:NE2	2:B:319:TYR:OH	2.31	0.61
1:C:325:LEU:HD13	1:C:331:HIS:CE1	2.35	0.61
2:H:221:GLN:O	2:H:225:ARG:HG3	2.01	0.61
2:D:210:GLY:O	2:D:214:LYS:HG2	2.00	0.61
1:E:315:HIS:O	1:E:318:ILE:HG13	2.01	0.61
1:G:431:LYS:HZ3	1:G:442:ILE:HB	1.64	0.61
2:F:300:THR:HG23	2:F:311:ILE:HD13	1.82	0.61
1:A:328:THR:OG1	1:A:330:LEU:HD23	2.01	0.61
1:A:455:LEU:HB3	2:B:281:ARG:HH21	1.64	0.61
2:B:320:ASN:C	2:B:320:ASN:HD22	2.03	0.61
2:D:320:ASN:C	2:D:320:ASN:HD22	2.03	0.61
2:F:292:ALA:O	2:F:296:MET:HG3	2.01	0.61
1:E:282:TRP:HZ3	1:E:375:LEU:HD22	1.66	0.60
1:E:306:ASN:HD22	1:E:306:ASN:N	1.97	0.60
2:F:262:SER:O	2:F:266:ILE:HG13	2.01	0.60
2:B:330:GLN:HG2	2:B:422:GLN:OE1	2.00	0.60
1:C:431:LYS:O	1:C:434:GLU:HB2	2.01	0.60
2:H:312:THR:HG22	2:H:318:SER:HA	1.82	0.60
2:B:214:LYS:O	2:B:217:ALA:HB3	2.01	0.60
1:G:431:LYS:NZ	1:G:442:ILE:HB	2.16	0.60
1:G:227:ASN:O	1:G:231:PRO:HA	2.01	0.60
1:A:227:ASN:HD21	1:A:232:VAL:CG2	2.13	0.60
1:E:316:ARG:NH1	1:E:325:LEU:O	2.34	0.60
1:E:383:LEU:HD21	1:E:389:VAL:HG21	1.84	0.60
2:F:230:ARG:HD3	2:F:314:LEU:HD22	1.83	0.60
2:F:356:LEU:O	2:F:360:ILE:HG13	2.01	0.59
2:B:248:ARG:NH1	2:B:248:ARG:HB3	2.17	0.59
1:E:454:MET:CE	2:F:263:VAL:HG12	2.27	0.59
1:G:234:ARG:O	1:G:237:GLU:HB2	2.02	0.59
2:D:230:ARG:HH11	2:D:314:LEU:HD23	1.67	0.59
2:H:428:LEU:HD22	2:H:428:LEU:H	1.68	0.59
2:H:289:LYS:HZ3	2:H:440:ILE:HA	1.67	0.59
2:B:230:ARG:HG2	2:B:230:ARG:HH11	1.68	0.59
2:F:302:ARG:HH21	2:F:354:PHE:HB3	1.67	0.59
2:F:312:THR:HG22	2:F:318:SER:CB	2.33	0.59
2:B:393:ILE:O	2:B:396:PRO:HD3	2.01	0.59
1:C:446:PRO:HB3	2:D:443:VAL:HG23	1.83	0.59
1:G:421:ARG:CA	1:G:421:ARG:HE	2.15	0.59
1:A:359:ASP:C	1:A:361:GLN:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:LEU:O	1:C:357:MET:HG3	2.02	0.59
1:G:264:PRO:CG	1:G:336:SER:HB3	2.32	0.59
2:H:254:HIS:HE2	2:H:319:TYR:HH	1.48	0.59
2:H:400:LEU:C	2:H:403:PRO:HD2	2.22	0.59
2:H:212:ILE:O	2:H:215:LEU:HB2	2.03	0.59
1:E:406:HIS:O	1:E:409:PRO:HD3	2.04	0.58
2:H:330:GLN:O	2:H:334:ILE:HG13	2.02	0.58
2:B:248:ARG:HH12	2:B:431:LYS:CE	2.15	0.58
2:B:441:TRP:O	2:B:443:VAL:N	2.36	0.58
1:G:447:ILE:HD12	1:G:447:ILE:N	2.18	0.58
2:F:324:PHE:HD1	2:F:329:LEU:HD12	1.67	0.58
1:G:294:LEU:O	1:G:298:VAL:HG23	2.03	0.58
1:A:320:VAL:HG22	1:A:321:LYS:N	2.18	0.58
2:B:237:PRO:HB3	2:B:250:GLN:NE2	2.19	0.58
2:B:400:LEU:C	2:B:403:PRO:HD2	2.24	0.58
2:D:400:LEU:O	2:D:404:ARG:HG3	2.03	0.58
2:F:330:GLN:HG2	2:F:422:GLN:HE22	1.67	0.58
2:B:378:ARG:NH1	2:B:378:ARG:HB3	2.13	0.58
2:D:356:LEU:HD13	2:D:387:LEU:HA	1.86	0.58
1:A:436:LEU:O	1:A:436:LEU:HD23	2.04	0.58
2:B:210:GLY:O	2:B:214:LYS:HE2	2.04	0.58
1:E:353:LEU:O	1:E:357:MET:HG3	2.04	0.57
1:E:437:PHE:O	1:E:441:LEU:HB2	2.04	0.57
2:F:406:LEU:O	2:F:409:LEU:HB2	2.04	0.57
2:B:427:ARG:NH2	1:E:273:ASP:OD1	2.37	0.57
2:H:219:GLN:NE2	2:H:302:ARG:HH12	2.03	0.57
2:H:321:ARG:HG3	2:H:338:PHE:CE2	2.38	0.57
2:B:219:GLN:HG2	2:B:269:PHE:CE1	2.39	0.57
2:F:293:ILE:HG22	5:F:7:HOH:O	2.04	0.57
2:D:309:GLU:OE1	2:D:321:ARG:NH2	2.37	0.57
2:F:395:HIS:N	2:F:396:PRO:HD3	2.20	0.57
2:D:243:GLN:HE21	1:G:294:LEU:HD23	1.68	0.57
1:C:302:ARG:NH1	2:H:330:GLN:HE22	1.97	0.57
2:H:394:ASN:HD22	2:H:395:HIS:CE1	2.22	0.57
2:B:243:GLN:HG3	2:B:248:ARG:CD	2.35	0.57
2:D:237:PRO:HG3	2:D:250:GLN:OE1	2.05	0.57
1:C:397:TYR:OH	2:D:407:MET:HG3	2.05	0.57
2:F:330:GLN:O	2:F:334:ILE:HG13	2.04	0.57
1:C:357:MET:CG	1:C:362:MET:HE3	2.35	0.57
1:E:306:ASN:O	1:E:310:ILE:HG13	2.05	0.57
2:D:240:PRO:O	2:D:241:ASP:HB3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLU:O	1:A:397:TYR:HB2	2.05	0.56
2:H:237:PRO:HG3	2:H:250:GLN:HB3	1.86	0.56
2:D:237:PRO:HG2	2:D:250:GLN:HB3	1.87	0.56
2:D:251:ARG:HH11	2:D:251:ARG:HG2	1.70	0.56
1:A:338:HIS:ND1	1:A:343:GLY:HA3	2.21	0.56
1:A:422:LEU:HD12	2:B:407:MET:HE1	1.87	0.56
1:C:236:LEU:HD22	1:C:240:LEU:CD2	2.36	0.56
2:D:281:ARG:HD2	2:D:284:GLN:HE22	1.70	0.56
2:B:418:VAL:O	2:B:421:GLU:HB2	2.05	0.56
2:B:438:SER:O	2:B:442:ASP:HB2	2.05	0.56
2:B:315:LYS:O	2:B:316:ASP:HB2	2.05	0.56
1:C:236:LEU:O	1:C:240:LEU:HD22	2.06	0.56
1:C:356:LYS:HG3	1:C:421:ARG:NH1	2.21	0.56
2:D:212:ILE:O	2:D:216:VAL:HG23	2.06	0.56
2:D:292:ALA:O	2:D:296:MET:HG3	2.06	0.56
1:E:441:LEU:HD12	1:E:442:ILE:H	1.71	0.56
2:F:363:PHE:CE1	2:F:379:LEU:HD13	2.41	0.56
2:B:233:VAL:HA	2:B:257:GLU:OE2	2.06	0.55
2:F:289:LYS:NZ	2:F:443:VAL:HG11	2.20	0.55
2:H:321:ARG:HG3	2:H:338:PHE:CD2	2.41	0.55
1:C:448:ASP:O	1:C:452:MET:HG3	2.06	0.55
2:D:221:GLN:HA	2:D:224:ARG:NH1	2.22	0.55
1:A:407:LYS:HA	1:A:407:LYS:HE2	1.88	0.55
1:C:437:PHE:HD2	1:C:438:PHE:CD2	2.24	0.55
1:G:264:PRO:O	1:G:267:ASN:HB2	2.07	0.55
1:A:410:GLU:OE2	1:A:410:GLU:N	2.34	0.55
2:B:293:ILE:HG23	2:B:294:GLU:N	2.22	0.55
2:B:374:LEU:HB3	2:B:378:ARG:NH2	2.21	0.55
2:F:290:THR:O	2:F:290:THR:HG22	2.06	0.55
2:F:315:LYS:O	2:F:316:ASP:HB2	2.07	0.55
2:H:219:GLN:HG2	2:H:269:PHE:CE1	2.41	0.55
1:A:225:SER:HB3	1:A:228:GLU:CD	2.27	0.55
1:C:333:HIS:CD2	1:C:334:ARG:N	2.73	0.55
2:F:270:ALA:HA	2:F:273:LEU:HD12	1.88	0.55
1:G:231:PRO:CG	1:G:234:ARG:HD3	2.37	0.55
2:F:402:PHE:HB3	2:F:403:PRO:CD	2.37	0.55
1:G:337:ALA:HB1	1:G:342:VAL:HG23	1.89	0.55
2:H:320:ASN:ND2	2:H:322:GLU:HB3	2.18	0.55
2:H:375:GLN:CB	2:H:378:ARG:HH21	2.19	0.55
1:A:263:ASP:HB2	1:A:264:PRO:HD2	1.88	0.54
2:H:305:ASN:ND2	2:H:312:THR:HG23	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PHE:CE2	2:B:403:PRO:HG3	2.39	0.54
1:C:310:ILE:HA	1:C:313:PHE:CE2	2.42	0.54
2:D:315:LYS:HA	2:D:315:LYS:HE3	1.90	0.54
1:A:349:VAL:HG22	1:A:428:ILE:HD13	1.89	0.54
2:F:300:THR:CG2	2:F:311:ILE:HD13	2.37	0.54
1:G:397:TYR:OH	2:H:407:MET:HG3	2.08	0.54
1:A:315:HIS:O	1:A:318:ILE:HG13	2.08	0.54
2:D:221:GLN:HE22	2:D:225:ARG:HH21	1.56	0.54
1:E:230:MET:SD	1:E:287:PRO:HB2	2.48	0.54
1:G:359:ASP:O	1:G:361:GLN:HG3	2.06	0.54
2:D:342:ARG:HH11	2:D:342:ARG:HB3	1.72	0.54
2:B:243:GLN:CD	2:B:248:ARG:HE	2.11	0.54
2:D:387:LEU:HD11	2:D:405:MET:HE1	1.90	0.54
1:G:378:PRO:HG3	1:G:390:GLU:HG2	1.89	0.54
2:H:218:ALA:HB2	2:H:272:GLN:HG2	1.89	0.54
2:H:263:VAL:O	2:H:267:VAL:HG23	2.08	0.54
2:H:372:ASP:O	2:H:376:VAL:HG23	2.08	0.54
2:H:439:GLU:O	2:H:439:GLU:HG2	2.07	0.54
1:A:369:CYS:O	1:A:373:ILE:HG13	2.08	0.54
2:B:256:THR:O	2:B:260:ILE:HG12	2.07	0.54
2:B:203:GLN:HG2	2:B:204:LEU:N	2.23	0.53
2:D:283:ASP:OD2	2:D:371:GLN:HB3	2.07	0.53
2:F:243:GLN:O	2:F:245:ARG:N	2.42	0.53
1:G:359:ASP:C	1:G:361:GLN:H	2.11	0.53
2:B:333:PHE:CZ	2:B:337:ILE:HD11	2.43	0.53
1:E:274:LYS:O	1:E:277:PHE:HD1	1.91	0.53
2:F:267:VAL:HG22	2:F:288:LEU:HD13	1.90	0.53
2:F:375:GLN:CD	2:F:378:ARG:HH21	2.12	0.53
1:G:422:LEU:HD12	2:H:407:MET:CE	2.38	0.53
1:G:306:ASN:HD22	1:G:433:LEU:HD11	1.74	0.53
2:D:333:PHE:C	2:D:336:PRO:HD2	2.28	0.53
2:F:342:ARG:O	2:F:345:ASN:HB3	2.09	0.53
1:E:406:HIS:ND1	1:E:407:LYS:N	2.56	0.53
2:F:401:MET:O	2:F:405:MET:HG3	2.07	0.53
2:H:251:ARG:HD2	2:H:326:LYS:O	2.08	0.53
1:G:441:LEU:HD21	2:H:443:VAL:HG21	1.91	0.53
1:A:338:HIS:CE1	1:A:343:GLY:HA3	2.42	0.53
2:B:304:TYR:CE1	2:B:342:ARG:HA	2.44	0.53
2:B:426:LEU:C	2:B:428:LEU:H	2.12	0.53
1:A:411:GLN:HE22	1:A:414:ARG:HH11	1.57	0.53
2:D:332:GLU:CD	2:D:332:GLU:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:ARG:HA	1:E:421:ARG:NE	2.24	0.53
1:G:231:PRO:HG3	1:G:234:ARG:HD3	1.90	0.53
2:H:320:ASN:O	2:H:324:PHE:HD2	1.92	0.53
1:E:356:LYS:HE3	2:F:377:GLU:OE2	2.08	0.53
2:B:263:VAL:O	2:B:267:VAL:HG23	2.09	0.53
1:E:268:ILE:HA	1:E:326:LEU:HD21	1.91	0.53
2:H:237:PRO:HB2	2:H:251:ARG:CZ	2.39	0.53
2:B:222:CYS:SG	2:B:268:ASP:HB3	2.49	0.52
2:D:431:LYS:O	2:D:432:LYS:HD3	2.10	0.52
1:C:406:HIS:O	1:C:409:PRO:HD3	2.09	0.52
2:D:320:ASN:ND2	2:D:323:ASP:H	2.08	0.52
2:H:255:PHE:HE1	4:H:104:L05:H23	1.75	0.52
2:H:329:LEU:N	2:H:329:LEU:HD22	2.24	0.52
1:A:231:PRO:HB2	1:A:234:ARG:HG2	1.90	0.52
2:D:240:PRO:O	2:D:241:ASP:CB	2.57	0.52
2:D:222:CYS:SG	2:D:268:ASP:HB3	2.50	0.52
2:D:291:SER:O	2:D:295:VAL:HG23	2.09	0.52
2:D:358:ILE:O	2:D:362:ILE:HG13	2.08	0.52
1:A:271:ALA:HB2	1:A:326:LEU:HD12	1.90	0.52
1:C:317:SER:O	1:C:320:VAL:HG12	2.08	0.52
1:C:230:MET:HE2	1:C:396:VAL:HG22	1.91	0.52
1:G:345:ILE:HA	1:G:348:ARG:HG3	1.90	0.52
2:D:317:PHE:H	2:D:317:PHE:HD2	1.57	0.52
1:G:283:ALA:HB1	1:G:289:PHE:CE2	2.45	0.52
2:H:224:ARG:C	2:H:226:SER:H	2.13	0.52
2:B:305:ASN:HB3	2:B:308:SER:HB3	1.92	0.52
1:G:242:VAL:HG11	1:G:282:TRP:HB2	1.91	0.52
1:G:345:ILE:HD13	1:G:431:LYS:HG2	1.91	0.52
2:H:244:SER:O	2:H:248:ARG:HB2	2.10	0.52
2:H:311:ILE:HD12	2:H:311:ILE:N	2.25	0.51
2:D:266:ILE:HG12	2:D:295:VAL:HG11	1.91	0.51
2:B:414:THR:O	2:B:418:VAL:HG23	2.10	0.51
1:E:279:LEU:HD11	1:E:309:LEU:HD13	1.91	0.51
1:E:348:ARG:HG2	1:E:348:ARG:HH11	1.76	0.51
1:A:453:GLU:O	1:A:456:GLU:N	2.38	0.51
2:F:241:ASP:CG	2:F:242:PRO:HD2	2.31	0.51
2:H:244:SER:HB3	2:H:247:ALA:HB3	1.92	0.51
1:G:419:LEU:HD22	2:H:407:MET:HE3	1.92	0.51
1:C:320:VAL:HG22	1:C:321:LYS:N	2.26	0.51
1:E:236:LEU:HD22	1:E:240:LEU:HD22	1.92	0.51
2:D:313:PHE:CE1	4:D:102:L05:H13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:360:ILE:HG23	2:D:380:GLN:HE21	1.75	0.51
2:D:391:VAL:HG11	2:D:405:MET:HE1	1.93	0.51
2:F:205:SER:HB2	2:F:206:PRO:CD	2.41	0.51
2:B:230:ARG:HG2	2:B:230:ARG:NH1	2.26	0.51
1:C:306:ASN:O	1:C:310:ILE:HG13	2.11	0.51
2:F:324:PHE:O	2:F:329:LEU:HB2	2.11	0.51
2:H:330:GLN:HG2	2:H:422:GLN:OE1	2.10	0.51
1:A:236:LEU:CD1	1:A:240:LEU:HD22	2.40	0.51
1:A:306:ASN:HD22	1:A:306:ASN:N	2.08	0.51
2:D:243:GLN:NE2	1:G:294:LEU:N	2.56	0.51
2:D:317:PHE:CD2	2:D:317:PHE:N	2.77	0.51
1:E:454:MET:HE3	2:F:264:GLN:HA	1.93	0.51
1:A:326:LEU:N	1:A:326:LEU:CD2	2.74	0.51
1:E:236:LEU:O	1:E:240:LEU:HD22	2.11	0.51
1:E:409:PRO:HG2	1:E:410:GLU:H	1.75	0.51
1:G:446:PRO:C	1:G:447:ILE:HG13	2.30	0.51
2:H:405:MET:O	2:H:408:LYS:HB2	2.11	0.51
2:H:438:SER:O	2:H:442:ASP:HB2	2.11	0.51
1:A:225:SER:HB3	1:A:228:GLU:HB2	1.93	0.50
1:A:326:LEU:HD23	1:A:330:LEU:O	2.11	0.50
2:H:212:ILE:O	2:H:216:VAL:HG23	2.11	0.50
2:H:225:ARG:HH21	2:H:268:ASP:CB	2.19	0.50
1:A:334:ARG:HA	1:A:346:PHE:CE1	2.46	0.50
1:A:385:ASN:ND2	1:A:388:GLU:N	2.58	0.50
2:D:281:ARG:HD2	2:D:284:GLN:NE2	2.26	0.50
2:D:333:PHE:CZ	2:D:337:ILE:HD11	2.46	0.50
1:G:315:HIS:CB	1:G:367:LEU:HD22	2.41	0.50
2:H:428:LEU:HD22	2:H:428:LEU:N	2.25	0.50
2:D:400:LEU:HB2	2:D:404:ARG:HH12	1.76	0.50
2:H:387:LEU:HD11	2:H:405:MET:CE	2.42	0.50
1:A:326:LEU:HD21	1:A:332:VAL:HG23	1.92	0.50
1:A:356:LYS:NZ	2:B:377:GLU:OE1	2.44	0.50
1:C:385:ASN:ND2	1:C:388:GLU:H	2.10	0.50
1:G:357:MET:HE2	1:G:367:LEU:HD13	1.93	0.50
1:A:437:PHE:CZ	1:A:441:LEU:HD22	2.47	0.50
1:G:307:GLU:HG2	1:G:425:LEU:HG	1.93	0.50
2:H:230:ARG:HG2	2:H:230:ARG:O	2.11	0.50
2:H:298:LEU:HD21	2:H:357:LEU:HD23	1.92	0.50
1:A:444:ASP:O	1:A:446:PRO:N	2.44	0.50
2:B:294:GLU:CD	2:B:367:ARG:HH22	2.14	0.50
2:F:335:ASN:HB2	2:F:336:PRO:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:269:PHE:CE2	2:H:273:LEU:HD21	2.47	0.50
1:A:406:HIS:O	1:A:409:PRO:HD3	2.12	0.50
1:A:345:ILE:HD11	1:A:428:ILE:HG23	1.93	0.50
1:A:276:LEU:HD23	1:A:279:LEU:HD12	1.93	0.50
2:D:330:GLN:HB2	2:D:422:GLN:OE1	2.12	0.50
2:H:325:ALA:C	2:H:327:ALA:H	2.14	0.50
1:C:436:LEU:HD23	1:C:436:LEU:O	2.12	0.49
2:D:237:PRO:CG	2:D:250:GLN:HB3	2.42	0.49
2:D:402:PHE:N	2:D:403:PRO:HD2	2.26	0.49
2:H:356:LEU:HD13	2:H:387:LEU:CA	2.39	0.49
2:B:227:PHE:CD1	2:B:315:LYS:HG3	2.47	0.49
2:B:292:ALA:HB3	5:B:14:HOH:O	2.13	0.49
2:B:320:ASN:ND2	2:B:320:ASN:C	2.65	0.49
2:B:260:ILE:HG23	2:B:436:LEU:HD23	1.95	0.49
1:G:441:LEU:HD23	1:G:441:LEU:C	2.32	0.49
1:C:310:ILE:HA	1:C:313:PHE:CD2	2.48	0.49
2:D:320:ASN:HD22	2:D:323:ASP:H	1.60	0.49
1:C:451:LEU:HD12	2:D:285:ILE:HG23	1.94	0.49
2:F:205:SER:OG	2:F:208:GLN:HG3	2.12	0.49
2:H:224:ARG:HB2	2:H:224:ARG:NH1	2.27	0.49
1:A:230:MET:SD	1:A:287:PRO:HB2	2.52	0.49
2:F:360:ILE:HD13	2:F:384:VAL:HG22	1.94	0.49
2:B:322:GLU:OE2	2:B:326:LYS:HE3	2.13	0.49
1:C:230:MET:SD	1:C:287:PRO:HB2	2.53	0.49
2:D:313:PHE:HE1	4:D:102:L05:H13	1.77	0.49
2:D:401:MET:O	2:D:405:MET:HG3	2.12	0.49
2:F:387:LEU:HD21	2:F:405:MET:CE	2.42	0.49
1:G:381:LYS:H	1:G:381:LYS:HD2	1.78	0.49
2:B:294:GLU:OE2	2:B:367:ARG:NH1	2.45	0.49
1:C:306:ASN:HD22	1:C:306:ASN:H	1.61	0.49
2:D:308:SER:O	2:D:309:GLU:C	2.49	0.49
1:A:440:LYS:O	1:A:441:LEU:C	2.50	0.49
1:E:230:MET:HE1	1:E:235:ILE:HD11	1.93	0.49
1:G:236:LEU:O	1:G:240:LEU:HD22	2.13	0.49
2:H:238:ILE:HG13	2:H:239:ALA:N	2.21	0.49
1:E:227:ASN:ND2	1:E:232:VAL:HG13	2.28	0.48
1:G:230:MET:HE2	1:G:235:ILE:HD11	1.95	0.48
2:H:277:LEU:HA	2:H:284:GLN:NE2	2.28	0.48
2:H:364:SER:HB2	2:H:367:ARG:HD3	1.93	0.48
1:A:294:LEU:O	1:A:298:VAL:HG23	2.13	0.48
1:C:326:LEU:HB2	1:C:330:LEU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:221:GLN:NE2	2:D:225:ARG:HH21	2.11	0.48
2:D:232:ARG:HH11	2:D:232:ARG:HG3	1.78	0.48
1:E:296:ASP:OD2	1:E:384:SER:HB3	2.13	0.48
2:F:204:LEU:HG	2:F:393:ILE:HD12	1.95	0.48
1:G:366:GLU:HG2	1:G:418:LEU:HD11	1.95	0.48
2:H:219:GLN:O	2:H:223:ASN:HB2	2.13	0.48
2:D:335:ASN:HB2	2:D:336:PRO:HD3	1.96	0.48
1:G:325:LEU:HD13	1:G:331:HIS:NE2	2.26	0.48
2:D:237:PRO:HG2	2:D:250:GLN:HB2	1.94	0.48
1:C:437:PHE:HE1	1:G:272:ALA:HB3	1.78	0.48
1:G:264:PRO:HB3	1:G:332:VAL:HG13	1.96	0.48
2:H:290:THR:OG1	2:H:367:ARG:HG3	2.13	0.48
2:B:316:ASP:O	2:B:317:PHE:HB2	2.14	0.48
1:C:388:GLU:O	1:C:391:ALA:HB3	2.13	0.48
1:E:310:ILE:HA	1:E:313:PHE:CD2	2.49	0.48
2:B:237:PRO:HG3	2:B:250:GLN:CB	2.42	0.48
2:B:253:ALA:O	2:B:257:GLU:HG3	2.14	0.48
2:H:305:ASN:HD21	2:H:312:THR:CG2	2.23	0.48
1:A:225:SER:O	1:A:228:GLU:HG3	2.13	0.48
1:A:268:ILE:HA	1:A:326:LEU:HD11	1.95	0.48
2:B:294:GLU:OE2	2:B:367:ARG:NH2	2.47	0.48
2:D:344:MET:HB3	2:D:344:MET:HE2	1.81	0.48
2:D:216:VAL:HG22	2:D:352:ALA:HA	1.96	0.48
1:G:449:THR:HB	2:H:439:GLU:OE2	2.13	0.48
2:B:205:SER:HB3	2:B:208:GLN:HG3	1.96	0.47
2:B:248:ARG:CZ	1:E:294:LEU:HD23	2.44	0.47
2:B:387:LEU:HD11	2:B:405:MET:SD	2.53	0.47
2:D:312:THR:O	2:D:312:THR:HG23	2.14	0.47
1:E:422:LEU:HD12	2:F:407:MET:CE	2.43	0.47
2:F:282:GLU:CD	2:F:282:GLU:H	2.17	0.47
1:C:317:SER:O	1:C:318:ILE:C	2.53	0.47
1:C:449:THR:HG22	1:C:450:PHE:N	2.29	0.47
1:G:352:GLU:CD	2:H:366:ASP:HB3	2.33	0.47
1:A:227:ASN:ND2	1:A:232:VAL:HG22	2.27	0.47
1:A:376:PHE:O	1:A:378:PRO:HD3	2.14	0.47
1:C:418:LEU:O	1:C:421:ARG:HB2	2.14	0.47
2:B:427:ARG:HH22	1:E:273:ASP:CG	2.17	0.47
1:E:307:GLU:HG2	1:E:425:LEU:CG	2.38	0.47
2:D:437:LEU:HA	2:D:440:ILE:CD1	2.44	0.47
2:H:387:LEU:HD11	2:H:405:MET:HE1	1.96	0.47
1:A:326:LEU:HD22	1:A:326:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:230:MET:HG2	1:E:395:LYS:HB3	1.97	0.47
1:A:264:PRO:HG3	1:A:336:SER:OG	2.14	0.47
1:C:302:ARG:HH22	2:H:330:GLN:NE2	2.10	0.47
1:A:320:VAL:HG22	1:A:321:LYS:H	1.79	0.47
1:A:360:MET:O	1:A:361:GLN:C	2.53	0.47
1:A:345:ILE:HG12	1:A:431:LYS:HG2	1.96	0.47
2:D:332:GLU:N	2:D:332:GLU:CD	2.67	0.47
1:E:366:GLU:CD	1:E:414:ARG:HH21	2.17	0.47
2:D:243:GLN:HG3	1:G:294:LEU:HD23	1.96	0.47
1:G:316:ARG:HG2	1:G:316:ARG:NH1	2.29	0.47
2:H:224:ARG:CB	2:H:224:ARG:HH11	2.27	0.47
2:H:333:PHE:O	2:H:337:ILE:HG13	2.14	0.47
2:H:331:VAL:CG2	2:H:335:ASN:HD22	2.27	0.47
1:C:378:PRO:HG3	1:C:390:GLU:OE2	2.15	0.47
2:D:332:GLU:O	2:D:336:PRO:HG2	2.15	0.47
2:D:243:GLN:HG3	1:G:294:LEU:CD2	2.45	0.47
2:H:254:HIS:NE2	2:H:319:TYR:OH	2.41	0.47
1:A:385:ASN:HD22	1:A:388:GLU:CG	2.16	0.46
2:B:439:GLU:O	2:B:443:VAL:HG23	2.14	0.46
2:D:208:GLN:O	2:D:212:ILE:HG13	2.14	0.46
1:A:294:LEU:HD12	2:F:243:GLN:HA	1.97	0.46
1:G:394:GLU:HA	1:G:397:TYR:HD2	1.77	0.46
1:G:449:THR:HB	2:H:439:GLU:CD	2.35	0.46
2:D:314:LEU:HD12	2:D:317:PHE:CZ	2.50	0.46
1:C:416:ALA:HB2	2:D:402:PHE:HE2	1.79	0.46
1:E:448:ASP:HA	2:F:439:GLU:CD	2.35	0.46
1:G:442:ILE:HG12	1:G:443:GLY:N	2.30	0.46
2:H:237:PRO:CG	2:H:250:GLN:HB3	2.45	0.46
2:H:293:ILE:HG22	5:H:19:HOH:O	2.15	0.46
2:H:360:ILE:HG23	2:H:380:GLN:HE21	1.80	0.46
2:B:330:GLN:O	2:B:334:ILE:HG13	2.16	0.46
2:B:350:ASN:OD1	2:B:350:ASN:C	2.54	0.46
2:H:219:GLN:HG2	2:H:269:PHE:HE1	1.80	0.46
1:A:239:GLU:OE2	1:A:282:TRP:NE1	2.49	0.46
2:B:208:GLN:O	2:B:211:MET:N	2.48	0.46
1:G:422:LEU:N	1:G:423:PRO:HD2	2.30	0.46
1:A:236:LEU:HD13	1:A:240:LEU:HD22	1.96	0.46
2:D:339:GLU:OE2	2:D:342:ARG:NH1	2.41	0.46
2:D:350:ASN:O	2:D:351:ASP:C	2.54	0.46
2:D:289:LYS:HG2	2:D:440:ILE:HA	1.97	0.46
1:A:435:HIS:CD2	1:A:435:HIS:N	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:303:ARG:HG3	2:H:303:ARG:HH11	1.81	0.46
1:C:457:ALA:O	2:D:271:LYS:NZ	2.49	0.46
2:F:276:PHE:CE2	2:F:284:GLN:HG2	2.50	0.46
1:G:441:LEU:HD21	2:H:443:VAL:CG2	2.45	0.46
2:D:314:LEU:CB	2:D:317:PHE:HE2	2.29	0.45
1:E:230:MET:N	1:E:231:PRO:HD3	2.30	0.45
1:A:236:LEU:HD13	1:A:236:LEU:C	2.37	0.45
2:H:312:THR:HG22	2:H:318:SER:CA	2.45	0.45
1:A:306:ASN:HD22	1:A:306:ASN:H	1.63	0.45
2:B:401:MET:HG3	2:B:405:MET:HE3	1.99	0.45
2:D:333:PHE:O	2:D:336:PRO:HD2	2.16	0.45
1:G:378:PRO:HD2	1:G:393:ARG:NH1	2.31	0.45
1:G:333:HIS:CD2	1:G:335:ASN:H	2.34	0.45
1:G:409:PRO:HG2	1:G:410:GLU:H	1.81	0.45
2:B:299:GLU:CD	2:B:302:ARG:HH21	2.20	0.45
2:D:320:ASN:ND2	2:D:320:ASN:C	2.70	0.45
2:H:224:ARG:C	2:H:226:SER:N	2.70	0.45
2:H:246:GLU:HA	2:H:246:GLU:OE2	2.16	0.45
2:B:202:VAL:HG22	2:B:203:GLN:N	2.31	0.45
2:F:368:PRO:HG2	5:F:9:HOH:O	2.15	0.45
2:D:241:ASP:N	2:D:242:PRO:HD3	2.25	0.45
2:D:263:VAL:O	2:D:267:VAL:HG23	2.17	0.45
2:D:205:SER:OG	2:D:208:GLN:HG3	2.17	0.45
2:D:314:LEU:HB2	2:D:317:PHE:HE2	1.82	0.45
2:F:303:ARG:HH11	2:F:303:ARG:HG3	1.81	0.45
2:D:363:PHE:CE1	2:D:379:LEU:HD13	2.52	0.45
2:H:360:ILE:HD13	2:H:384:VAL:HG22	1.98	0.45
1:A:268:ILE:HA	1:A:326:LEU:CD1	2.47	0.45
2:B:387:LEU:O	2:B:391:VAL:HG23	2.17	0.45
2:B:441:TRP:O	2:B:442:ASP:C	2.55	0.45
2:D:227:PHE:HA	2:D:230:ARG:HD2	1.98	0.45
1:E:307:GLU:CG	1:E:425:LEU:HG	2.40	0.45
2:F:301:SER:HB2	2:F:344:MET:HB2	1.98	0.45
2:D:427:ARG:NE	1:G:277:PHE:CE2	2.85	0.45
1:A:335:ASN:O	1:A:338:HIS:N	2.50	0.44
1:E:268:ILE:HA	1:E:326:LEU:CD2	2.47	0.44
1:E:409:PRO:HG2	1:E:410:GLU:N	2.32	0.44
2:F:230:ARG:CD	2:F:314:LEU:HB3	2.47	0.44
2:B:310:SER:OG	2:B:318:SER:HB2	2.17	0.44
2:B:423:VAL:O	2:B:426:LEU:HB2	2.17	0.44
2:D:427:ARG:HG2	2:D:427:ARG:H	1.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:437:LEU:HA	2:D:440:ILE:HD12	1.99	0.44
2:F:280:SER:OG	2:F:283:ASP:HB2	2.17	0.44
1:G:227:ASN:ND2	1:G:232:VAL:HG13	2.33	0.44
1:C:294:LEU:HD12	2:H:248:ARG:HE	1.82	0.44
2:H:300:THR:CG2	2:H:311:ILE:HG12	2.46	0.44
2:D:243:GLN:HE21	1:G:294:LEU:CD2	2.30	0.44
1:E:370:LEU:O	1:E:373:ILE:HB	2.17	0.44
2:H:264:GLN:HE21	2:H:264:GLN:C	2.21	0.44
2:H:333:PHE:CE2	2:H:337:ILE:HD11	2.53	0.44
2:H:298:LEU:CD2	2:H:357:LEU:HD23	2.47	0.44
1:G:349:VAL:HG22	1:G:428:ILE:HD13	2.00	0.44
1:G:276:LEU:O	1:G:276:LEU:HD23	2.17	0.44
1:G:321:LYS:H	1:G:321:LYS:HD3	1.82	0.44
1:G:404:CYS:SG	1:G:414:ARG:HG2	2.58	0.44
1:A:326:LEU:CD2	1:A:332:VAL:HG23	2.48	0.44
2:B:287:LEU:O	2:B:291:SER:CB	2.65	0.44
1:E:306:ASN:H	1:E:306:ASN:ND2	2.09	0.44
2:F:289:LYS:HZ1	2:F:443:VAL:HG11	1.82	0.44
1:G:404:CYS:SG	1:G:414:ARG:CG	3.05	0.44
1:A:381:LYS:CD	1:A:381:LYS:H	2.30	0.44
1:G:310:ILE:HA	1:G:313:PHE:CD2	2.51	0.44
1:G:367:LEU:O	1:G:371:ARG:HG3	2.18	0.44
2:H:219:GLN:NE2	2:H:358:ILE:HD12	2.32	0.44
2:B:427:ARG:C	2:B:428:LEU:HD22	2.37	0.44
2:H:325:ALA:C	2:H:327:ALA:N	2.72	0.44
2:H:331:VAL:CG2	2:H:335:ASN:ND2	2.81	0.44
1:E:441:LEU:HD12	1:E:442:ILE:N	2.33	0.43
2:F:275:GLY:HA3	2:F:379:LEU:HD21	2.00	0.43
2:F:290:THR:CG2	2:F:367:ARG:HD2	2.47	0.43
2:H:270:ALA:HA	2:H:273:LEU:HD12	1.98	0.43
1:C:416:ALA:HB2	2:D:402:PHE:CE2	2.53	0.43
1:G:227:ASN:O	1:G:231:PRO:CA	2.64	0.43
2:F:262:SER:HB2	4:F:103:L05:H13	1.99	0.43
1:A:231:PRO:HB2	1:A:234:ARG:CG	2.48	0.43
2:B:222:CYS:SG	2:B:268:ASP:CB	3.06	0.43
2:B:339:GLU:OE1	2:B:339:GLU:HA	2.19	0.43
2:B:341:SER:O	2:B:342:ARG:C	2.57	0.43
1:C:435:HIS:O	1:C:439:PHE:HB2	2.17	0.43
2:F:230:ARG:CD	2:F:314:LEU:HD13	2.47	0.43
2:D:430:ASP:HB2	1:G:280:VAL:HG11	2.00	0.43
1:G:437:PHE:CE1	2:H:445:GLU:OE2	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:347:LEU:HD23	2:H:347:LEU:HA	1.77	0.43
1:C:363:ASP:C	1:C:363:ASP:OD1	2.57	0.43
1:E:454:MET:HE1	2:F:264:GLN:HG2	1.99	0.43
2:F:311:ILE:HD12	2:F:324:PHE:CE2	2.54	0.43
1:G:445:THR:HA	1:G:446:PRO:HD3	1.75	0.43
2:D:360:ILE:HG23	2:D:380:GLN:NE2	2.34	0.43
1:C:444:ASP:O	2:D:443:VAL:HG21	2.18	0.43
1:A:411:GLN:NE2	1:A:414:ARG:HH11	2.17	0.43
2:D:312:THR:HA	2:D:318:SER:HA	1.99	0.43
2:D:342:ARG:CZ	2:D:342:ARG:HB3	2.47	0.43
1:C:426:ARG:NH1	2:D:414:THR:OG1	2.52	0.43
1:G:316:ARG:NH1	1:G:325:LEU:O	2.51	0.43
2:H:237:PRO:HG2	2:H:251:ARG:HG3	2.00	0.43
2:H:424:PHE:C	2:H:426:LEU:H	2.20	0.43
1:C:394:GLU:O	1:C:397:TYR:HB2	2.18	0.43
1:E:227:ASN:HD21	1:E:232:VAL:CG2	2.27	0.43
2:F:242:PRO:C	2:F:244:SER:H	2.21	0.43
2:F:315:LYS:NZ	2:F:315:LYS:HB2	2.34	0.43
1:G:453:GLU:OE2	1:G:454:MET:N	2.52	0.43
2:B:248:ARG:HB3	2:B:248:ARG:HH11	1.84	0.43
2:B:426:LEU:C	2:B:428:LEU:N	2.71	0.43
2:D:245:ARG:HH11	2:D:245:ARG:HG3	1.84	0.43
2:F:320:ASN:ND2	2:F:322:GLU:H	2.16	0.43
1:G:435:HIS:CD2	1:G:437:PHE:HB3	2.53	0.43
1:C:441:LEU:HD12	1:C:442:ILE:H	1.84	0.43
1:G:317:SER:OG	1:G:324:ILE:HA	2.18	0.43
1:C:421:ARG:NE	1:C:421:ARG:HA	2.34	0.42
2:F:311:ILE:HD12	2:F:324:PHE:CZ	2.54	0.42
1:G:446:PRO:C	1:G:447:ILE:CG1	2.86	0.42
1:E:296:ASP:O	1:E:300:LEU:HG	2.19	0.42
2:H:331:VAL:HG23	2:H:335:ASN:ND2	2.34	0.42
2:H:398:ASP:C	2:H:400:LEU:H	2.22	0.42
1:A:359:ASP:C	1:A:361:GLN:N	2.71	0.42
2:B:357:LEU:HD13	2:B:405:MET:HG2	2.00	0.42
2:B:259:ALA:HB3	2:B:437:LEU:HD11	2.01	0.42
1:C:230:MET:HE1	1:C:396:VAL:HG22	1.99	0.42
1:E:265:VAL:HG23	1:E:340:ALA:HB1	2.01	0.42
1:E:294:LEU:HD12	1:E:294:LEU:HA	1.78	0.42
2:F:230:ARG:HD2	2:F:314:LEU:HB3	2.00	0.42
1:G:313:PHE:C	1:G:313:PHE:CD1	2.92	0.42
2:H:222:CYS:SG	2:H:268:ASP:HB3	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:PRO:O	1:C:268:ILE:HG13	2.20	0.42
2:D:330:GLN:CA	2:D:330:GLN:NE2	2.77	0.42
1:G:415:PHE:HE2	2:H:403:PRO:HG3	1.83	0.42
2:H:333:PHE:C	2:H:336:PRO:HD2	2.39	0.42
2:H:335:ASN:O	2:H:339:GLU:HG3	2.19	0.42
2:H:304:TYR:CE1	2:H:342:ARG:HA	2.54	0.42
2:H:212:ILE:HD13	2:H:390:TYR:CD1	2.55	0.42
2:D:374:LEU:HD12	2:D:374:LEU:HA	1.85	0.42
1:E:318:ILE:CG2	1:E:358:ARG:HG3	2.48	0.42
1:E:307:GLU:OE1	1:E:426:ARG:HA	2.19	0.42
1:G:312:SER:OG	1:G:371:ARG:NH1	2.53	0.42
2:H:224:ARG:NH1	2:H:224:ARG:CB	2.83	0.42
2:H:294:GLU:CD	2:H:367:ARG:NH2	2.73	0.42
1:C:422:LEU:HD12	2:D:407:MET:HE1	1.98	0.42
2:H:288:LEU:HA	2:H:291:SER:OG	2.20	0.42
2:H:294:GLU:CD	2:H:367:ARG:HH22	2.22	0.42
2:H:363:PHE:CE1	2:H:379:LEU:HD13	2.54	0.42
1:A:359:ASP:O	1:A:361:GLN:N	2.52	0.42
1:C:376:PHE:HB3	1:C:393:ARG:HB2	2.01	0.42
2:H:236:TRP:HE3	2:H:254:HIS:CD2	2.38	0.42
2:H:260:ILE:HD11	2:H:434:PRO:HB2	2.00	0.42
2:H:335:ASN:HB2	2:H:336:PRO:HD3	2.01	0.42
2:H:375:GLN:HB2	2:H:378:ARG:NH2	2.26	0.42
2:H:419:HIS:ND1	5:H:37:HOH:O	2.26	0.42
1:A:234:ARG:NE	1:A:234:ARG:HA	2.34	0.42
2:B:243:GLN:NE2	2:B:248:ARG:HE	2.17	0.42
1:C:369:CYS:HB3	1:C:400:LEU:HD22	2.02	0.42
1:E:293:PRO:HB2	1:E:296:ASP:OD2	2.20	0.42
1:E:316:ARG:O	1:E:316:ARG:HG3	2.19	0.42
1:E:326:LEU:N	1:E:326:LEU:HD12	2.35	0.42
1:E:345:ILE:HD13	1:E:345:ILE:O	2.19	0.42
2:H:205:SER:OG	2:H:208:GLN:HG3	2.19	0.42
2:B:333:PHE:CE2	2:B:337:ILE:HD11	2.55	0.42
2:B:374:LEU:O	2:B:378:ARG:HG2	2.20	0.42
2:B:294:GLU:HG2	2:B:412:LEU:HB3	2.02	0.42
2:D:219:GLN:NE2	2:D:302:ARG:NH2	2.52	0.42
1:E:359:ASP:C	1:E:361:GLN:H	2.23	0.42
1:G:357:MET:HE2	1:G:362:MET:SD	2.60	0.42
1:A:263:ASP:HB2	1:A:264:PRO:CD	2.50	0.41
1:A:445:THR:O	1:A:445:THR:HG22	2.20	0.41
1:A:453:GLU:O	1:A:455:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:331:VAL:CG1	2:D:335:ASN:ND2	2.83	0.41
1:A:349:VAL:HG22	1:A:428:ILE:HG21	2.02	0.41
1:A:437:PHE:O	1:A:441:LEU:HB2	2.20	0.41
2:B:202:VAL:HG22	2:B:203:GLN:H	1.85	0.41
2:D:388:HIS:HB2	2:D:402:PHE:CZ	2.55	0.41
2:F:203:GLN:O	2:F:204:LEU:C	2.58	0.41
1:G:377:ASN:HA	1:G:378:PRO:HD2	1.94	0.41
1:G:451:LEU:HB3	2:H:285:ILE:HD12	2.03	0.41
2:H:387:LEU:CD2	2:H:405:MET:HE2	2.43	0.41
1:C:378:PRO:HD2	1:C:393:ARG:NH1	2.36	0.41
2:D:281:ARG:HA	2:D:284:GLN:NE2	2.35	0.41
1:E:230:MET:HE2	1:E:235:ILE:HD11	2.01	0.41
1:E:339:SER:C	1:E:341:GLY:H	2.23	0.41
2:H:417:SER:O	2:H:420:SER:HB3	2.20	0.41
1:A:444:ASP:O	1:A:445:THR:C	2.58	0.41
2:D:256:THR:O	2:D:260:ILE:HG13	2.20	0.41
2:D:300:THR:CG2	2:D:311:ILE:HG12	2.50	0.41
1:G:285:ARG:HD3	1:G:285:ARG:HA	1.91	0.41
1:G:406:HIS:C	1:G:406:HIS:CD2	2.94	0.41
1:A:317:SER:OG	1:A:324:ILE:HA	2.21	0.41
1:C:337:ALA:O	1:C:340:ALA:HB3	2.20	0.41
2:H:398:ASP:C	2:H:400:LEU:N	2.73	0.41
2:H:424:PHE:C	2:H:426:LEU:N	2.73	0.41
2:B:355:ALA:O	2:B:356:LEU:C	2.58	0.41
1:E:448:ASP:O	1:E:452:MET:HG3	2.20	0.41
1:G:356:LYS:CG	1:G:421:ARG:HH11	2.29	0.41
2:H:300:THR:HG22	2:H:311:ILE:HG12	2.02	0.41
1:A:238:ALA:HA	1:A:285:ARG:HD2	2.03	0.41
1:A:289:PHE:CD1	1:A:375:LEU:HD21	2.55	0.41
1:C:437:PHE:CD2	1:C:438:PHE:CD2	3.06	0.41
2:D:331:VAL:HG13	2:D:335:ASN:ND2	2.36	0.41
2:F:426:LEU:HD22	2:F:431:LYS:HG3	2.03	0.41
1:A:316:ARG:HD2	1:A:325:LEU:O	2.21	0.41
2:B:426:LEU:O	2:B:428:LEU:N	2.53	0.41
1:C:372:ALA:HB3	1:C:396:VAL:HG11	2.02	0.41
2:D:226:SER:OG	2:D:265:GLU:HG3	2.21	0.41
2:D:428:LEU:CD2	2:D:428:LEU:H	2.29	0.41
1:C:442:ILE:CD1	1:G:266:THR:HG21	2.51	0.41
2:D:330:GLN:HG2	1:G:302:ARG:NH1	2.35	0.41
2:H:207:GLU:HA	2:H:207:GLU:OE2	2.21	0.41
1:A:330:LEU:N	1:A:330:LEU:HD22	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:ASN:OD1	2:B:352:ALA:N	2.54	0.41
2:D:320:ASN:ND2	2:D:323:ASP:OD2	2.53	0.41
2:D:329:LEU:C	2:D:330:GLN:HE21	2.23	0.41
1:E:313:PHE:C	1:E:313:PHE:CD1	2.94	0.41
2:F:330:GLN:HB2	2:F:422:GLN:OE1	2.21	0.41
2:H:331:VAL:HG13	2:H:332:GLU:N	2.35	0.41
1:A:326:LEU:HD21	1:A:332:VAL:CG2	2.50	0.41
2:B:364:SER:O	2:B:367:ARG:HG2	2.21	0.41
2:B:371:GLN:HA	2:B:371:GLN:NE2	2.36	0.41
1:E:306:ASN:ND2	1:E:306:ASN:N	2.67	0.41
1:E:341:GLY:O	1:E:440:LYS:HE2	2.21	0.41
2:F:209:LEU:HD13	2:F:209:LEU:C	2.42	0.41
2:F:314:LEU:HB2	2:F:317:PHE:HD2	1.85	0.41
2:H:259:ALA:O	2:H:262:SER:HB3	2.20	0.41
1:A:225:SER:HB3	1:A:228:GLU:OE2	2.20	0.41
1:E:337:ALA:HB1	1:E:342:VAL:HG23	2.03	0.41
2:F:230:ARG:HA	2:F:233:VAL:HG23	2.03	0.41
2:F:255:PHE:O	2:F:258:LEU:HB2	2.21	0.41
2:H:236:TRP:CH2	2:H:251:ARG:HB3	2.56	0.41
2:H:313:PHE:O	2:H:317:PHE:HB2	2.21	0.41
1:A:342:VAL:O	1:A:342:VAL:HG23	2.21	0.40
2:F:353:GLU:OE2	2:F:390:TYR:HE2	2.04	0.40
2:H:291:SER:O	2:H:292:ALA:C	2.59	0.40
2:H:203:GLN:HA	2:H:393:ILE:HD11	2.03	0.40
1:A:320:VAL:CG2	1:A:321:LYS:N	2.85	0.40
1:E:283:ALA:O	1:E:289:PHE:HB3	2.22	0.40
2:F:281:ARG:HG3	2:F:281:ARG:HH11	1.87	0.40
1:G:359:ASP:C	1:G:361:GLN:N	2.72	0.40
2:H:313:PHE:O	2:H:317:PHE:HD2	2.04	0.40
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.56	0.40
2:B:293:ILE:CG2	2:B:294:GLU:N	2.85	0.40
1:C:320:VAL:CG2	1:C:321:LYS:N	2.82	0.40
1:E:377:ASN:OD1	1:E:379:ASP:N	2.50	0.40
1:G:239:GLU:OE2	1:G:371:ARG:NE	2.53	0.40
1:G:439:PHE:O	1:G:442:ILE:HG22	2.20	0.40
2:H:333:PHE:CZ	2:H:337:ILE:HD11	2.57	0.40
2:B:333:PHE:O	2:B:337:ILE:HG13	2.20	0.40
1:C:338:HIS:NE2	1:C:347:ASP:OD2	2.54	0.40
1:E:348:ARG:HG2	1:E:348:ARG:NH1	2.36	0.40
2:H:215:LEU:O	2:H:218:ALA:N	2.55	0.40
1:E:310:ILE:HA	1:E:313:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/238 (88%)	181 (86%)	23 (11%)	6 (3%)	4	15
1	C	211/238 (89%)	191 (90%)	19 (9%)	1 (0%)	29	61
1	E	210/238 (88%)	189 (90%)	18 (9%)	3 (1%)	11	34
1	G	210/238 (88%)	185 (88%)	21 (10%)	4 (2%)	8	26
2	B	240/244 (98%)	206 (86%)	24 (10%)	10 (4%)	3	9
2	D	240/244 (98%)	220 (92%)	16 (7%)	4 (2%)	9	29
2	F	240/244 (98%)	209 (87%)	23 (10%)	8 (3%)	4	13
2	H	242/244 (99%)	206 (85%)	31 (13%)	5 (2%)	7	23
All	All	1803/1928 (94%)	1587 (88%)	175 (10%)	41 (2%)	6	21

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	441	LEU
1	A	454	MET
2	B	314	LEU
2	D	203	GLN
2	D	240	PRO
1	E	406	HIS
2	F	242	PRO
2	F	316	ASP
1	G	442	ILE
1	G	447	ILE
2	H	316	ASP
2	B	230	ARG
2	B	244	SER
2	B	315	LYS

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Mol	Chain	Res	Type
2	B	442	ASP
1	C	354	VAL
2	D	241	ASP
1	E	407	LYS
2	F	207	GLU
2	F	244	SER
1	G	354	VAL
1	G	443	GLY
1	A	360	MET
1	A	445	THR
1	A	453	GLU
2	B	209	LEU
2	B	427	ARG
2	B	435	PRO
2	D	242	PRO
1	E	231	PRO
2	F	204	LEU
2	F	235	PRO
2	F	237	PRO
2	F	206	PRO
2	H	326	LYS
2	H	430	ASP
2	H	435	PRO
1	A	361	GLN
2	B	425	ALA
2	H	431	LYS
2	B	393	ILE

### 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	182/205 (89%)	171 (94%)	11 (6%)	19	48
1	C	183/205 (89%)	172 (94%)	11 (6%)	19	48
1	E	182/205 (89%)	167 (92%)	15 (8%)	11	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	182/205 (89%)	170 (93%)	12 (7%)	16	44
2	B	219/221 (99%)	201 (92%)	18 (8%)	11	33
2	D	219/221 (99%)	204 (93%)	15 (7%)	16	42
2	F	219/221 (99%)	208 (95%)	11 (5%)	24	56
2	H	221/221 (100%)	213 (96%)	8 (4%)	35	69
All	All	1607/1704 (94%)	1506 (94%)	101 (6%)	18	46

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	LEU
1	A	276	LEU
1	A	280	VAL
1	A	306	ASN
1	A	309	LEU
1	A	326	LEU
1	A	345	ILE
1	A	381	LYS
1	A	383	LEU
1	A	407	LYS
1	A	444	ASP
2	B	214	LYS
2	B	224	ARG
2	B	230	ARG
2	B	250	GLN
2	B	255	PHE
2	B	262	SER
2	B	281	ARG
2	B	309	GLU
2	B	312	THR
2	B	317	PHE
2	B	320	ASN
2	B	375	GLN
2	B	377	GLU
2	B	378	ARG
2	B	388	HIS
2	B	416	SER
2	B	435	PRO
2	B	442	ASP
1	C	232	VAL

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Mol	Chain	Res	Type
1	C	236	LEU
1	C	240	LEU
1	C	279	LEU
1	C	306	ASN
1	C	316	ARG
1	C	326	LEU
1	C	350	LEU
1	C	383	LEU
1	C	444	ASP
1	C	451	LEU
2	D	238	ILE
2	D	243	GLN
2	D	255	PHE
2	D	281	ARG
2	D	290	THR
2	D	293	ILE
2	D	316	ASP
2	D	317	PHE
2	D	320	ASN
2	D	330	GLN
2	D	354	PHE
2	D	385	GLU
2	D	398	ASP
2	D	435	PRO
2	D	440	ILE
1	E	229	ASP
1	E	236	LEU
1	E	240	LEU
1	E	285	ARG
1	E	306	ASN
1	E	309	LEU
1	E	313	PHE
1	E	345	ILE
1	E	390	GLU
1	E	393	ARG
1	E	426	ARG
1	E	444	ASP
1	E	451	LEU
1	E	454	MET
1	E	456	GLU
2	F	220	GLN
2	F	237	PRO

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Mol	Chain	Res	Type
2	F	241	ASP
2	F	243	GLN
2	F	246	GLU
2	F	281	ARG
2	F	282	GLU
2	F	315	LYS
2	F	351	ASP
2	F	374	LEU
2	F	428	LEU
1	G	236	LEU
1	G	240	LEU
1	G	263	ASP
1	G	266	THR
1	G	274	LYS
1	G	276	LEU
1	G	313	PHE
1	G	321	LYS
1	G	348	ARG
1	G	351	THR
1	G	426	ARG
1	G	447	ILE
2	H	255	PHE
2	H	264	GLN
2	H	281	ARG
2	H	366	ASP
2	H	367	ARG
2	H	429	GLN
2	H	432	LYS
2	H	435	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	275	GLN
1	A	306	ASN
1	A	333	HIS
1	A	385	ASN
1	A	406	HIS
1	A	411	GLN
1	A	435	HIS
2	B	221	GLN

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Mol	Chain	Res	Type
2	B	223	ASN
2	B	305	ASN
2	B	320	ASN
2	B	330	GLN
2	B	345	ASN
2	B	371	GLN
1	C	227	ASN
1	C	270	GLN
1	C	306	ASN
1	C	331	HIS
1	C	333	HIS
1	C	335	ASN
1	C	385	ASN
2	D	219	GLN
2	D	221	GLN
2	D	243	GLN
2	D	249	GLN
2	D	284	GLN
2	D	305	ASN
2	D	320	ASN
2	D	330	GLN
2	D	335	ASN
2	D	380	GLN
1	E	227	ASN
1	E	267	ASN
1	E	275	GLN
1	E	306	ASN
1	E	335	ASN
2	F	219	GLN
2	F	249	GLN
2	F	305	ASN
2	F	335	ASN
2	F	345	ASN
2	F	371	GLN
2	F	419	HIS
1	G	227	ASN
1	G	267	ASN
1	G	270	GLN
1	G	306	ASN
1	G	333	HIS
1	G	335	ASN
1	G	361	GLN

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Mol	Chain	Res	Type
1	G	406	HIS
1	G	435	HIS
2	H	219	GLN
2	H	249	GLN
2	H	264	GLN
2	H	305	ASN
2	H	320	ASN
2	H	330	GLN
2	H	380	GLN
2	H	394	ASN
2	H	429	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	L05	B	101	-	32,32,32	1.72	8 (25%)	40,44,44	0.87	1 (2%)
4	L05	H	104	-	32,32,32	1.65	11 (34%)	40,44,44	0.87	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	REA	G	501	-	19,22,22	1.64	3 (15%)	26,30,30	1.23	3 (11%)
4	L05	F	103	-	32,32,32	1.77	12 (37%)	40,44,44	0.88	2 (5%)
3	REA	E	504	-	19,22,22	1.68	3 (15%)	26,30,30	1.18	2 (7%)
3	REA	A	502	-	19,22,22	2.06	5 (26%)	26,30,30	1.20	2 (7%)
4	L05	D	102	-	32,32,32	1.59	8 (25%)	40,44,44	0.86	1 (2%)
3	REA	C	503	-	19,22,22	1.79	4 (21%)	26,30,30	1.39	3 (11%)

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	L05	B	101	-	-	2/14/34/34	0/4/4/4
4	L05	H	104	-	-	2/14/34/34	0/4/4/4
3	REA	G	501	-	-	2/13/32/32	0/1/1/1
4	L05	F	103	-	-	2/14/34/34	0/4/4/4
3	REA	E	504	-	-	2/13/32/32	0/1/1/1
3	REA	A	502	-	-	2/13/32/32	0/1/1/1
4	L05	D	102	-	-	2/14/34/34	0/4/4/4
3	REA	C	503	-	-	2/13/32/32	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	REA	C1-C6	5.97	1.62	1.53
3	C	503	REA	C1-C6	4.83	1.60	1.53
3	G	501	REA	C1-C6	4.34	1.59	1.53
3	E	504	REA	C1-C6	3.98	1.59	1.53
3	E	504	REA	C5-C6	3.43	1.40	1.34
3	C	503	REA	C5-C6	3.23	1.40	1.34
3	A	502	REA	C5-C6	3.22	1.40	1.34
4	F	103	L05	C5-C6	3.19	1.44	1.39
3	G	501	REA	C5-C6	3.01	1.39	1.34
4	B	101	L05	C5-C6	2.94	1.44	1.39
4	D	102	L05	C5-C6	2.73	1.43	1.39
4	F	103	L05	C19-C14	2.68	1.44	1.38
4	B	101	L05	C23-C22	2.62	1.43	1.39
4	D	102	L05	C23-C22	2.61	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	104	L05	C5-C6	2.56	1.43	1.39
4	B	101	L05	C27-C22	2.56	1.43	1.39
4	D	102	L05	C29-C3	2.55	1.43	1.38
4	F	103	L05	C23-C22	2.54	1.43	1.39
4	F	103	L05	C27-C22	2.53	1.43	1.39
4	H	104	L05	C19-C14	2.51	1.44	1.38
4	B	101	L05	C15-C14	2.48	1.44	1.38
4	D	102	L05	C29-C28	2.45	1.43	1.38
4	F	103	L05	C5-C4	2.42	1.43	1.38
4	H	104	L05	C23-C22	2.41	1.43	1.39
4	B	101	L05	C19-C14	2.39	1.44	1.38
4	D	102	L05	C27-C22	2.38	1.43	1.39
4	F	103	L05	C29-C3	2.36	1.43	1.38
4	F	103	L05	C28-C6	2.35	1.43	1.39
4	F	103	L05	C29-C28	2.31	1.43	1.38
4	B	101	L05	C4-C3	2.28	1.43	1.38
4	F	103	L05	C15-C14	2.27	1.43	1.38
3	G	501	REA	C20-C13	2.25	1.55	1.50
4	H	104	L05	C29-C28	2.22	1.42	1.38
3	C	503	REA	C20-C13	2.22	1.55	1.50
4	D	102	L05	C19-C14	2.21	1.43	1.38
4	H	104	L05	C27-C22	2.18	1.43	1.39
4	F	103	L05	C8-N7	2.18	1.41	1.35
4	B	101	L05	C29-C3	2.17	1.43	1.38
4	B	101	L05	C29-C28	2.15	1.42	1.38
4	H	104	L05	C15-C14	2.15	1.43	1.38
3	A	502	REA	C18-C5	2.13	1.54	1.50
3	A	502	REA	C20-C13	2.13	1.55	1.50
4	D	102	L05	C18-C19	2.12	1.43	1.38
4	H	104	L05	C16-C15	2.12	1.43	1.38
3	E	504	REA	C20-C13	2.12	1.55	1.50
4	F	103	L05	C16-C15	2.12	1.43	1.38
4	H	104	L05	C28-C6	2.12	1.42	1.39
4	H	104	L05	C29-C3	2.10	1.42	1.38
4	D	102	L05	C28-C6	2.09	1.42	1.39
3	A	502	REA	C19-C9	2.08	1.55	1.50
3	C	503	REA	C14-C13	2.08	1.37	1.35
4	F	103	L05	C4-C3	2.03	1.42	1.38
4	H	104	L05	C18-C19	2.01	1.43	1.38
4	H	104	L05	C8-N7	2.01	1.40	1.35

All (15) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	REA	C18-C5-C6	4.27	129.32	124.53
3	A	502	REA	C18-C5-C6	3.68	128.66	124.53
3	E	504	REA	C18-C5-C6	3.49	128.44	124.53
3	G	501	REA	C18-C5-C6	3.37	128.31	124.53
4	D	102	L05	O11-C10-C9	-2.76	124.64	128.99
4	F	103	L05	O11-C10-C9	-2.69	124.74	128.99
3	G	501	REA	C18-C5-C4	-2.62	108.58	113.62
4	B	101	L05	O11-C10-C9	-2.58	124.91	128.99
3	E	504	REA	C18-C5-C4	-2.50	108.81	113.62
4	H	104	L05	O11-C10-C9	-2.48	125.06	128.99
3	C	503	REA	C18-C5-C4	-2.41	108.98	113.62
3	C	503	REA	C7-C8-C9	2.37	129.82	126.23
4	F	103	L05	C6-N7-C8	2.19	133.47	127.78
3	G	501	REA	C7-C8-C9	2.16	129.50	126.23
3	A	502	REA	C18-C5-C4	-2.06	109.65	113.62

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	101	L05	C29-C3-O2-C1
4	F	103	L05	C4-C3-O2-C1
4	D	102	L05	C4-C3-O2-C1
4	B	101	L05	C4-C3-O2-C1
4	H	104	L05	C4-C3-O2-C1
4	F	103	L05	C29-C3-O2-C1
4	D	102	L05	C29-C3-O2-C1
4	H	104	L05	C29-C3-O2-C1
3	G	501	REA	C11-C10-C9-C19
3	E	504	REA	C11-C10-C9-C19
3	A	502	REA	C11-C10-C9-C19
3	C	503	REA	C11-C10-C9-C19
3	G	501	REA	C11-C10-C9-C8
3	E	504	REA	C11-C10-C9-C8
3	A	502	REA	C11-C10-C9-C8
3	C	503	REA	C11-C10-C9-C8

There are no ring outliers.

3 monomers are involved in 4 short contacts:

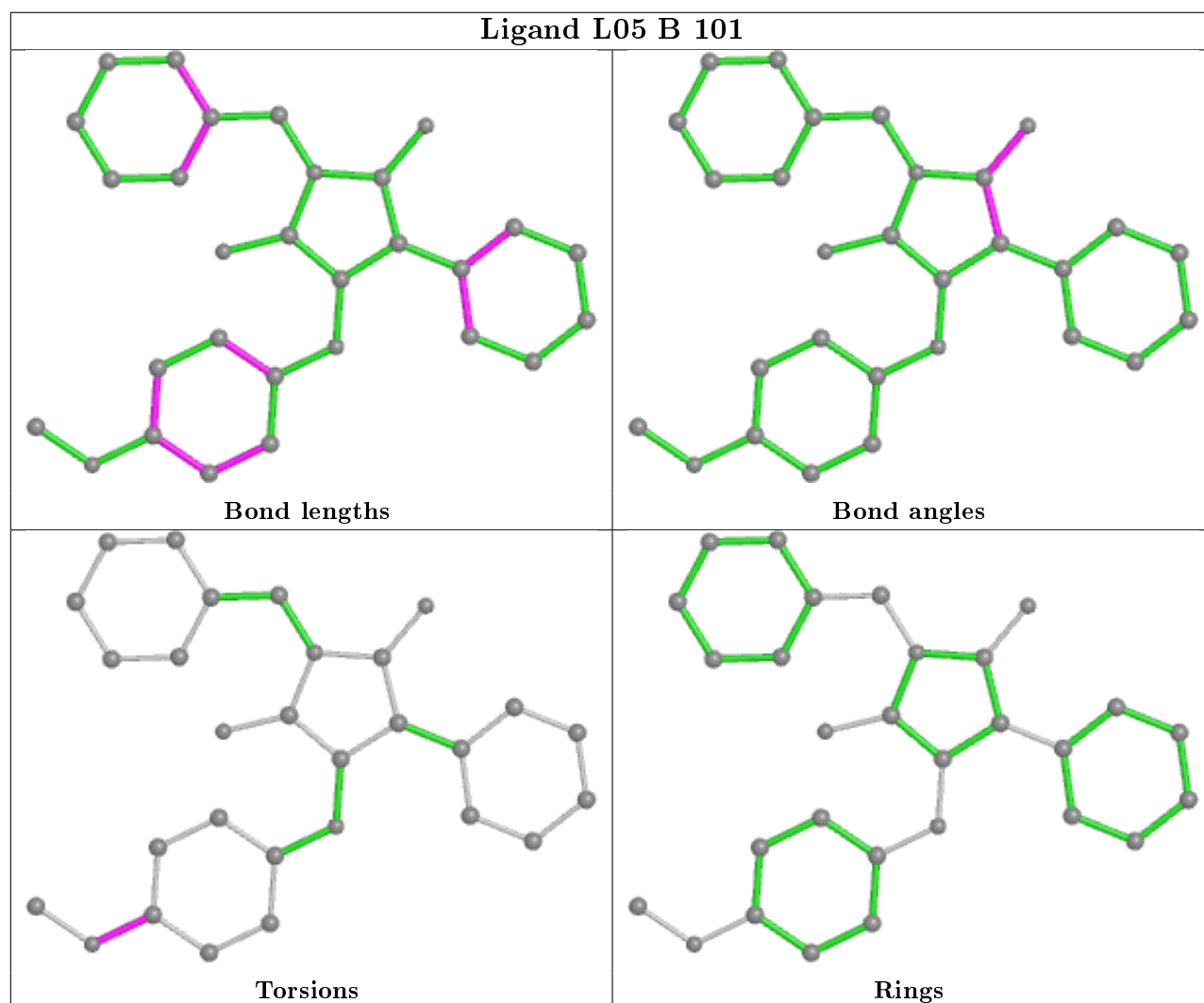
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	104	L05	1	0

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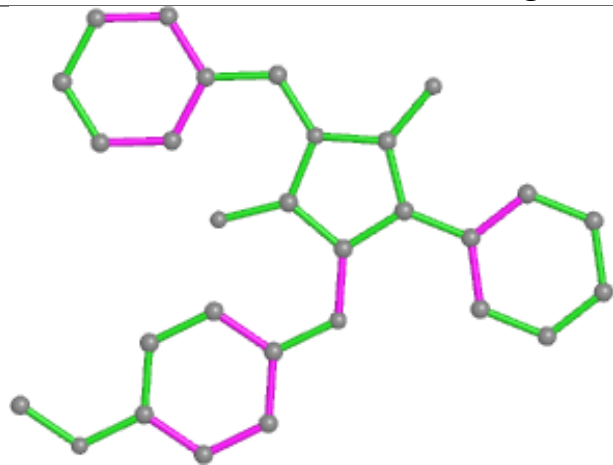
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	103	L05	1	0
4	D	102	L05	2	0

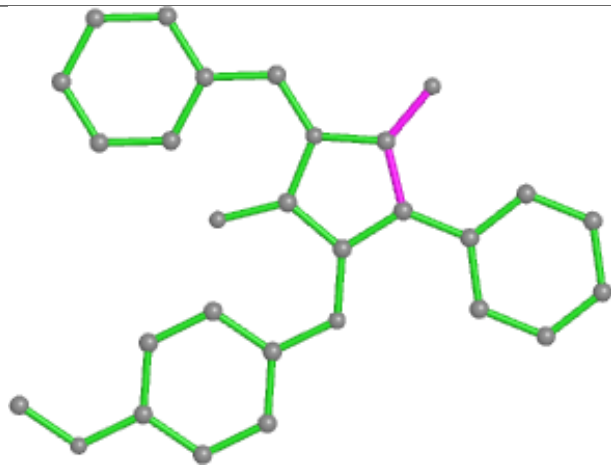
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



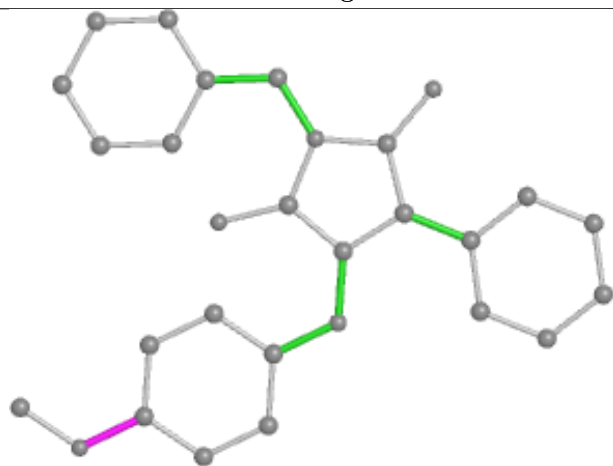
## Ligand L05 H 104



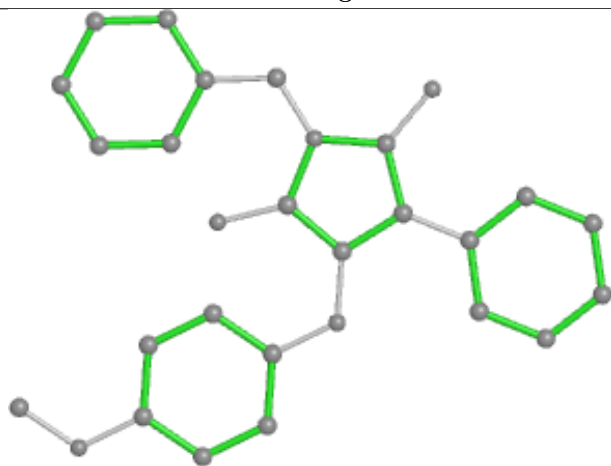
Bond lengths



Bond angles

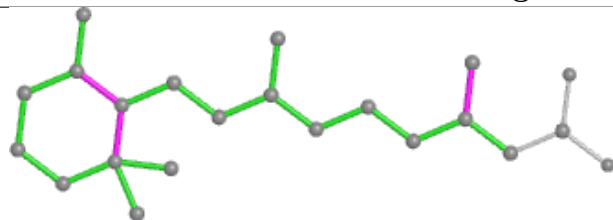


Torsions

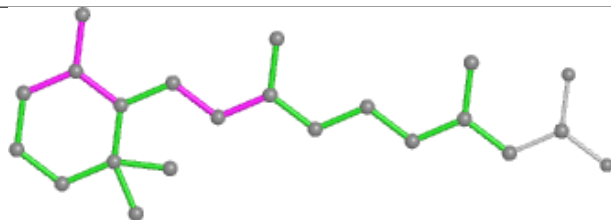


Rings

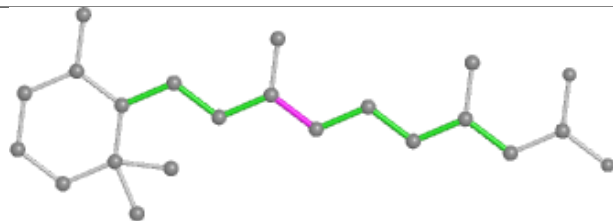
## Ligand REA G 501



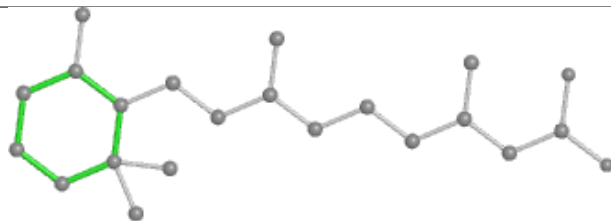
Bond lengths



Bond angles

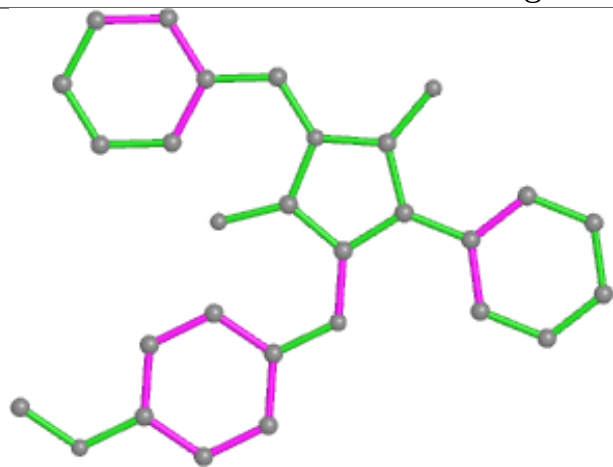


Torsions

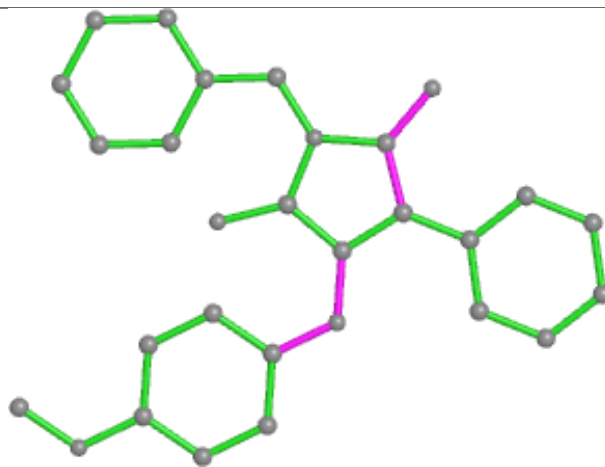


Rings

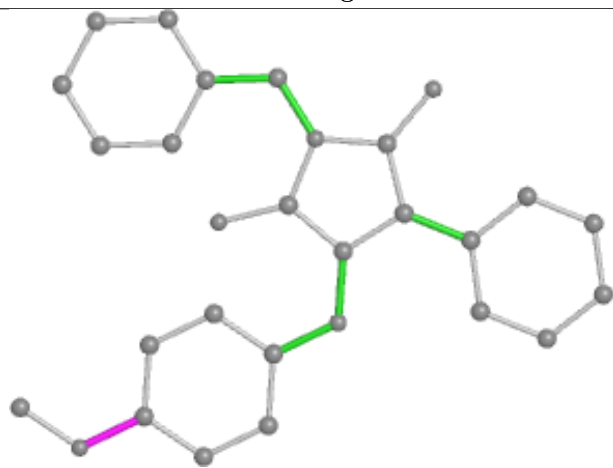
## Ligand L05 F 103



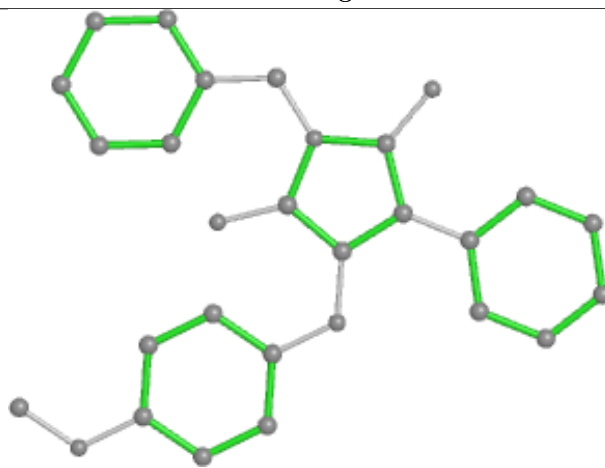
Bond lengths



Bond angles

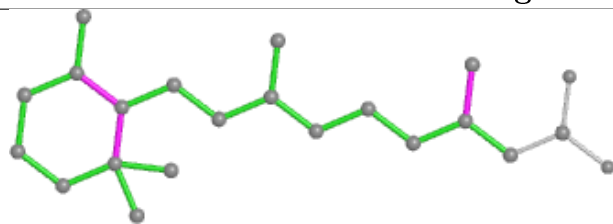


Torsions

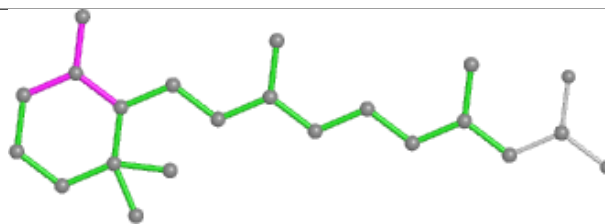


Rings

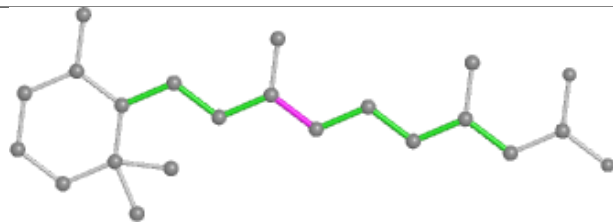
## Ligand REA E 504



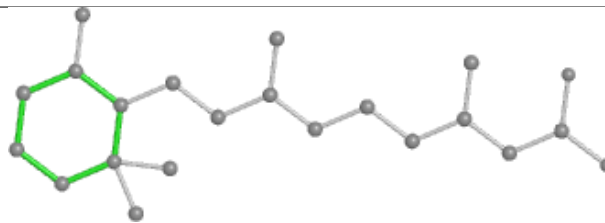
Bond lengths



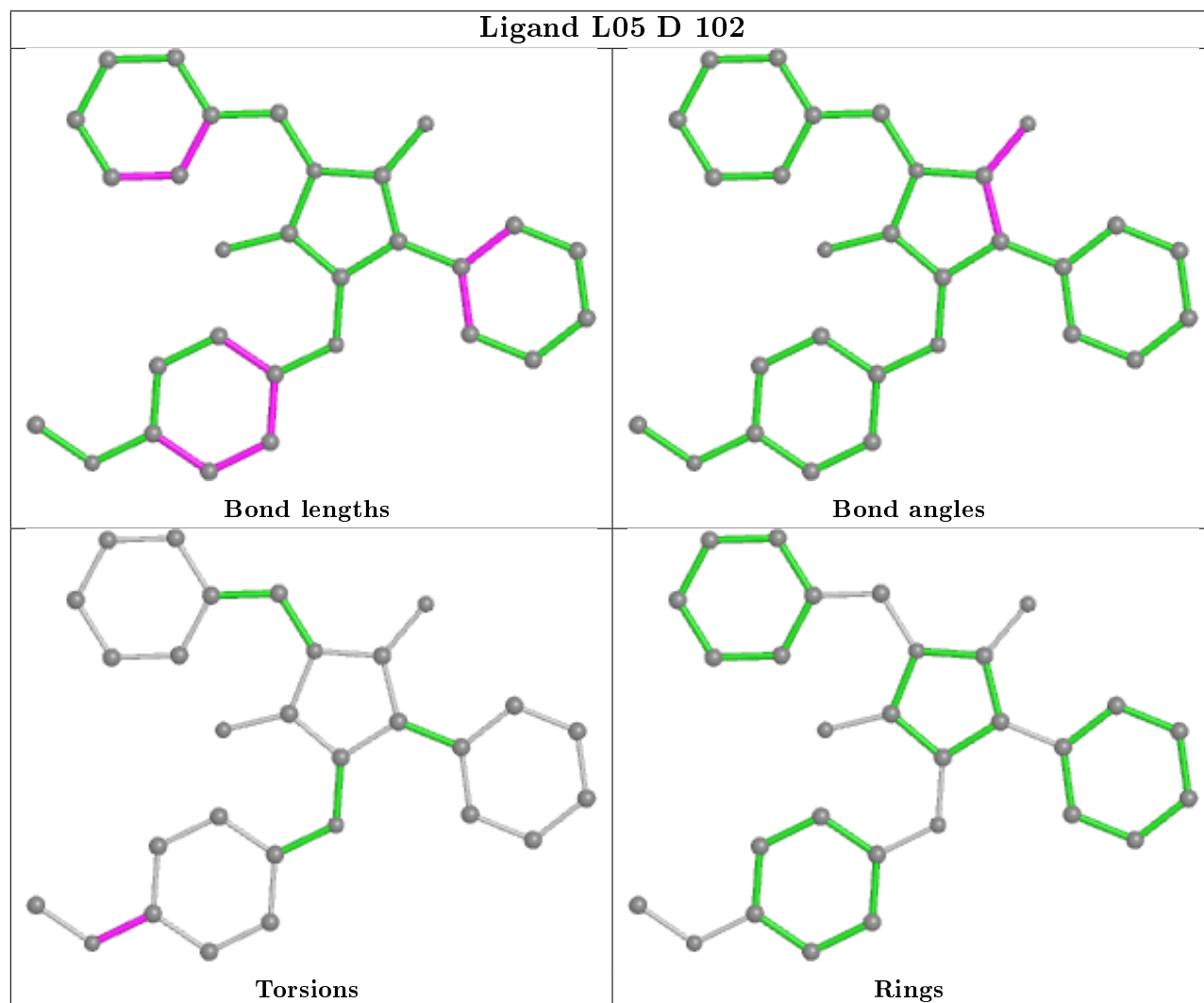
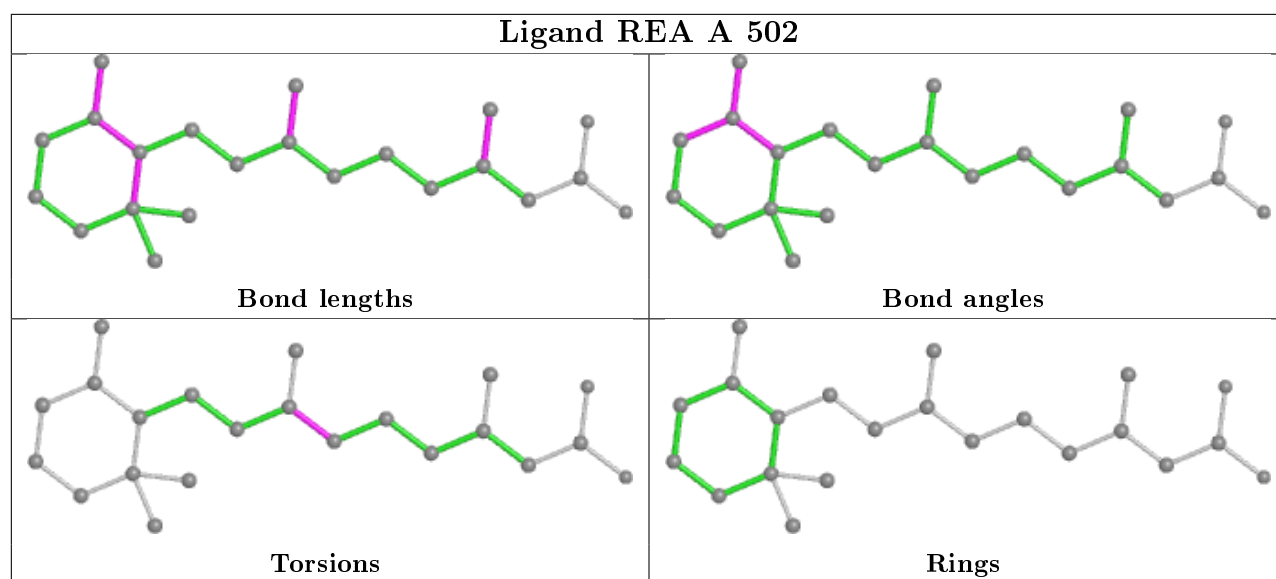
Bond angles

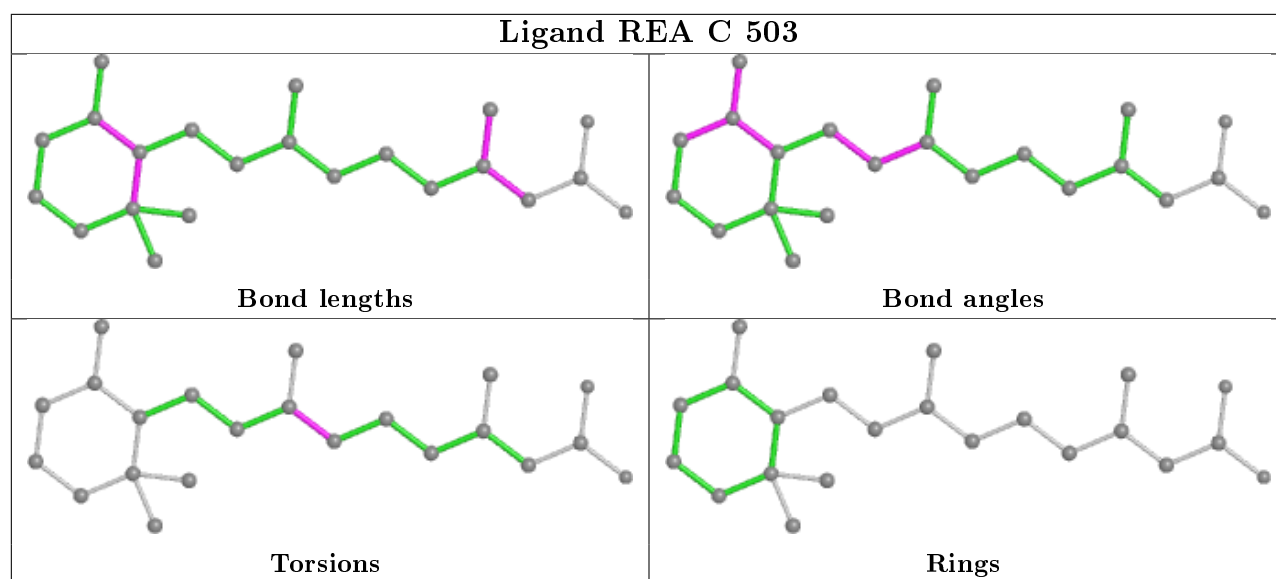


Torsions



Rings





## 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	214/238 (89%)	-0.39	2 (0%) 84 80	12, 33, 58, 84	0
1	C	215/238 (90%)	-0.60	0 100 100	9, 28, 48, 54	0
1	E	214/238 (89%)	-0.47	0 100 100	16, 36, 54, 64	0
1	G	214/238 (89%)	-0.31	3 (1%) 75 70	15, 37, 61, 82	0
2	B	242/244 (99%)	-0.30	5 (2%) 63 54	13, 36, 76, 99	0
2	D	242/244 (99%)	-0.44	1 (0%) 92 91	9, 30, 64, 90	0
2	F	242/244 (99%)	-0.14	9 (3%) 41 31	16, 40, 100, 110	0
2	H	244/244 (100%)	-0.13	10 (4%) 37 27	21, 43, 94, 104	0
All	All	1827/1928 (94%)	-0.34	30 (1%) 72 66	9, 36, 76, 110	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	202	VAL	6.0
1	A	442	ILE	5.0
2	D	202	VAL	4.9
2	H	231	LEU	4.6
1	A	443	GLY	4.3
2	B	231	LEU	4.0
1	G	442	ILE	3.9
1	G	443	GLY	3.5
2	H	242	PRO	3.4
2	H	397	HIS	3.3
2	F	315	LYS	2.9
2	B	241	ASP	2.9
2	F	231	LEU	2.8
2	H	245	ARG	2.7
2	B	315	LYS	2.6
2	H	236	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	237	PRO	2.5
2	H	315	LYS	2.5
2	F	235	PRO	2.4
2	F	230	ARG	2.3
2	B	238	ILE	2.3
2	F	242	PRO	2.2
1	G	384	SER	2.2
2	H	230	ARG	2.2
2	H	243	GLN	2.1
2	F	236	TRP	2.0
2	B	232	ARG	2.0
2	F	227	PHE	2.0
2	F	228	SER	2.0
2	H	228	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

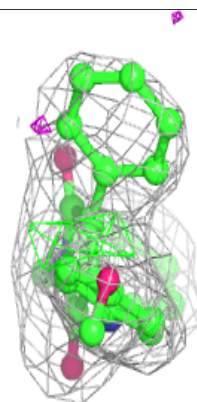
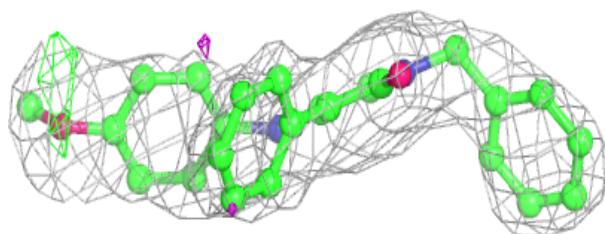
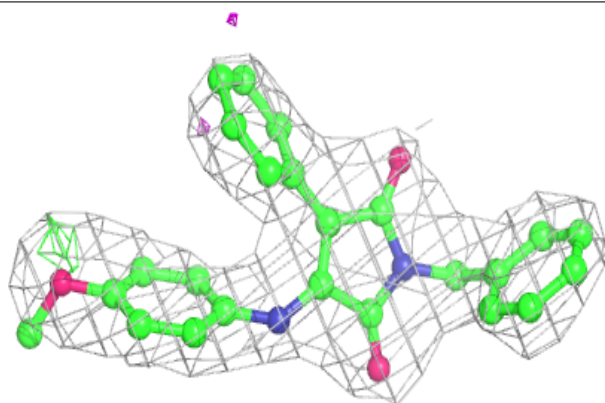
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	L05	F	103	29/29	0.93	0.20	37,42,49,52	0
4	L05	H	104	29/29	0.94	0.17	30,35,43,49	0
3	REA	A	502	22/22	0.94	0.19	23,28,31,32	0
3	REA	E	504	22/22	0.95	0.17	11,16,23,25	0
3	REA	G	501	22/22	0.95	0.17	11,20,25,26	0
3	REA	C	503	22/22	0.95	0.17	6,19,20,21	0
4	L05	D	102	29/29	0.96	0.16	8,14,21,24	0
4	L05	B	101	29/29	0.96	0.14	22,25,31,32	0



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

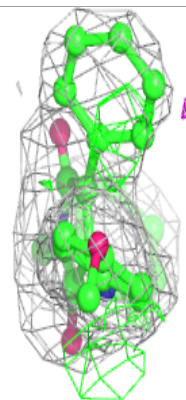
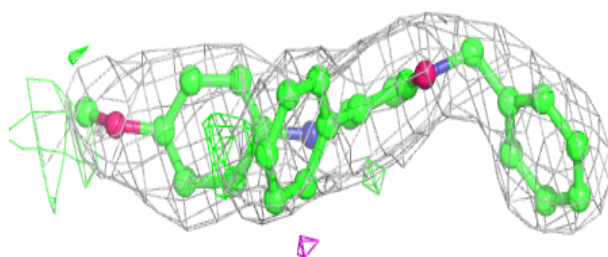
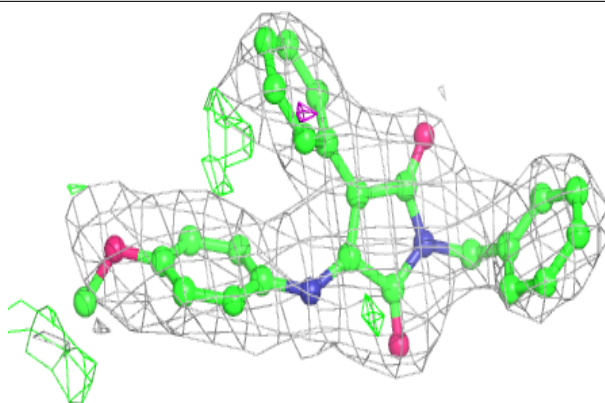
**Electron density around L05 F 103:**

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

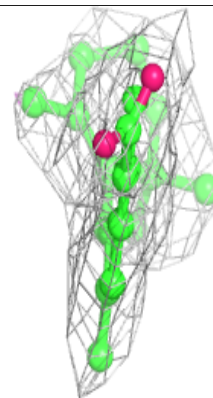
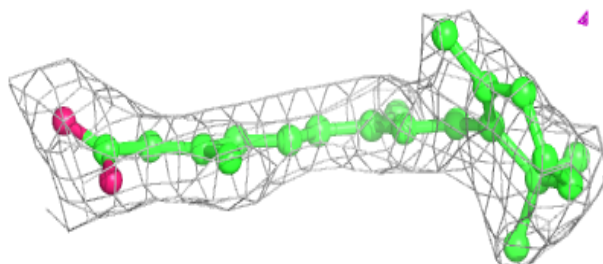
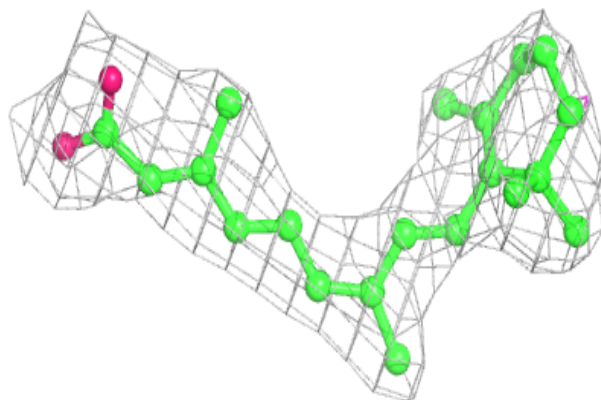


**Electron density around L05 H 104:**

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

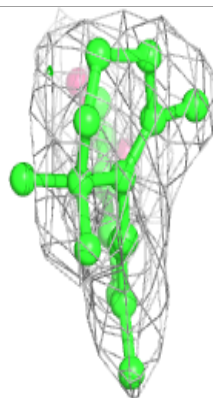
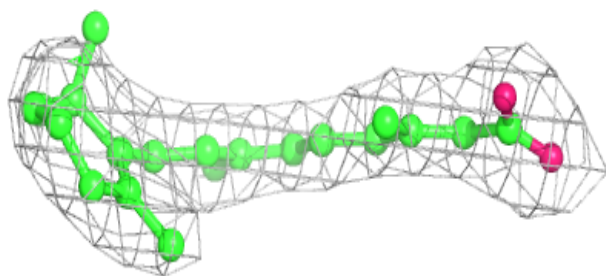
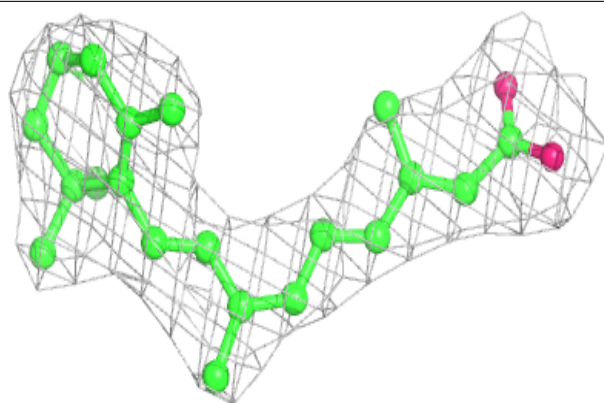
**Electron density around REA A 502:**

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

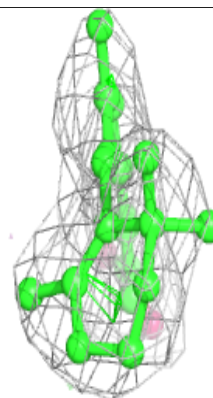
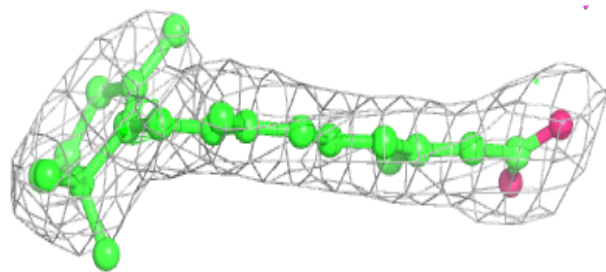
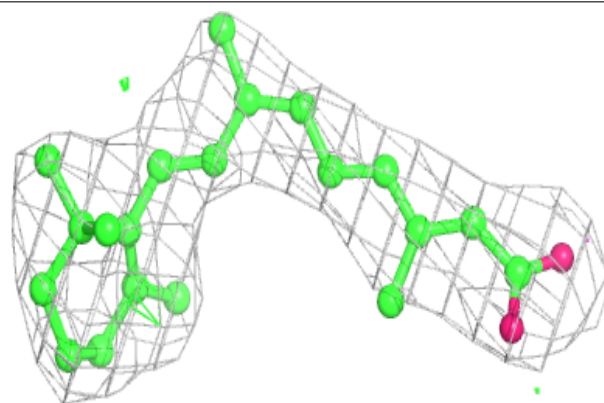


**Electron density around REA E 504:**

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

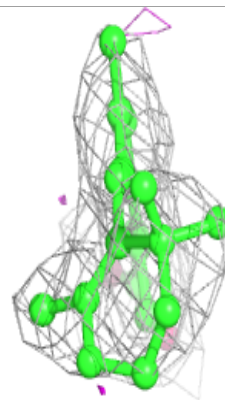
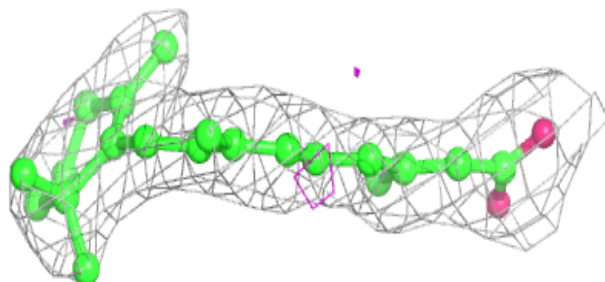
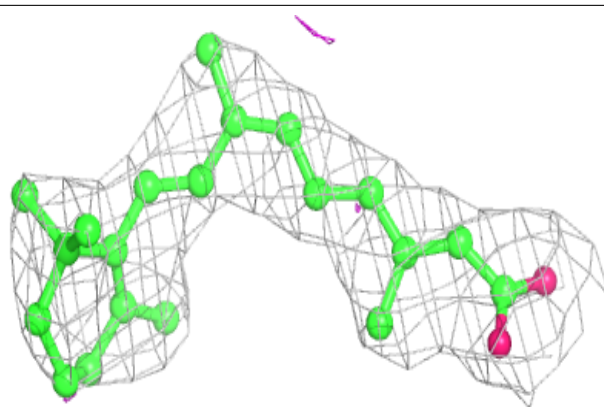
**Electron density around REA G 501:**

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

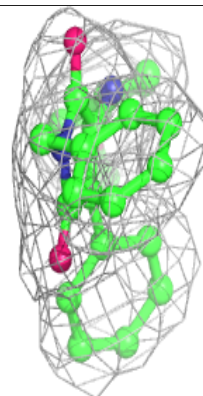
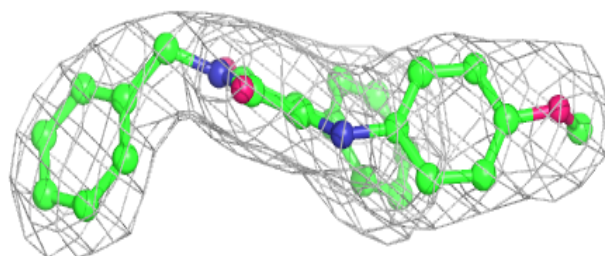
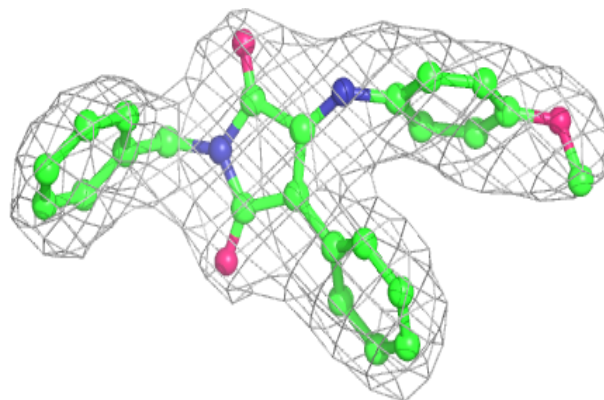


**Electron density around REA C 503:**

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

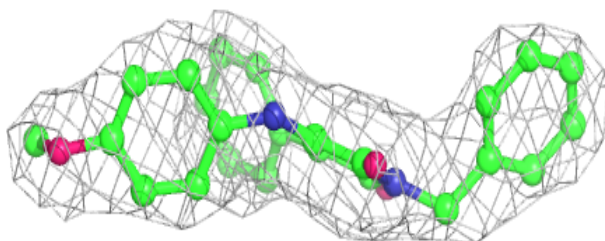
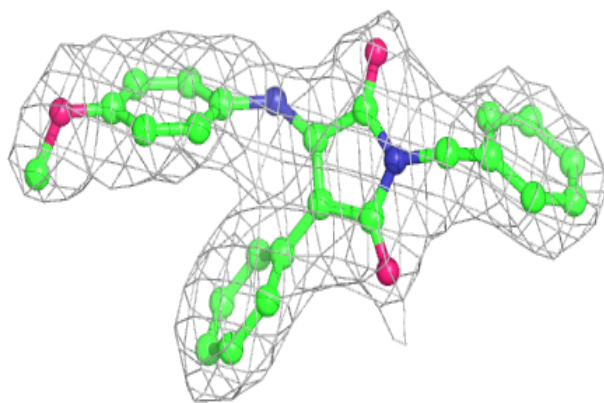
**Electron density around L05 D 102:**

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



**Electron density around L05 B 101:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.