



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:02 am BST

PDB ID : 3OB7  
Title : Human Thymidylate Synthase R163K with Cys 195 covalently modified by Glutathione  
Authors : Gibson, L.M.; Celeste, L.R.; Lovelace, L.L.; Lebioda, L.  
Deposited on : 2010-08-06  
Resolution : 2.75 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

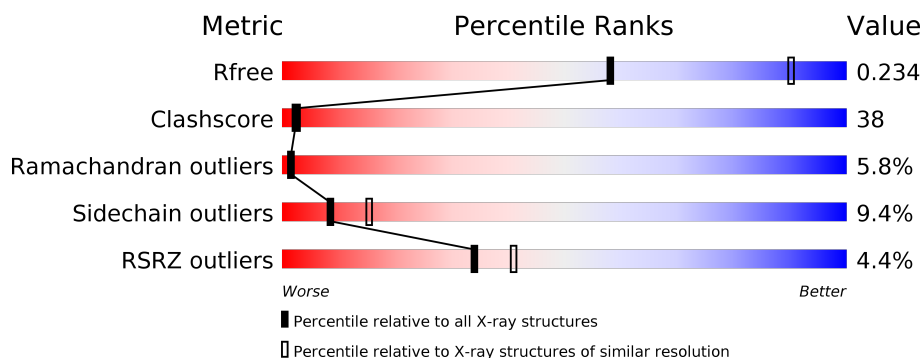
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	313	<div> <div>50%</div> <div>37%</div> <div>•</div> <div>10%</div> </div>
1	B	313	<div>4%</div> <div>40%</div> <div>41%</div> <div>9%</div> <div>10%</div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GSH	D	314	-	-	X	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11445 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.

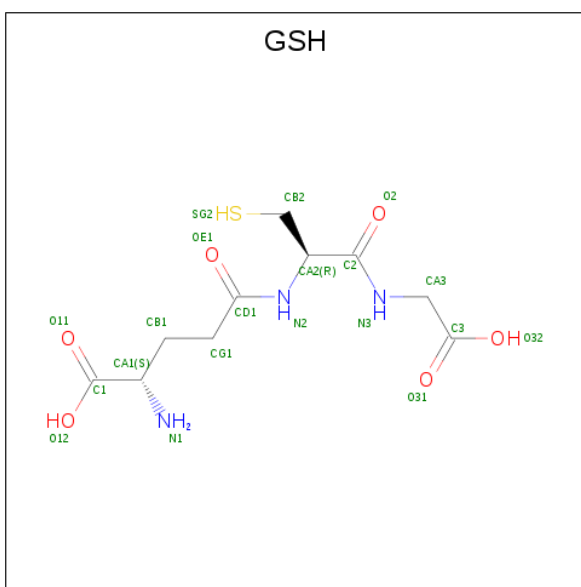
- Molecule 1 is a protein called Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	B	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	C	280	Total	C	N	O	S	0	0	0
			2261	1447	394	409	11			
1	D	281	Total	C	N	O	S	0	0	0
			2268	1451	395	411	11			
1	E	280	Total	C	N	O	S	0	0	0
			2261	1447	394	409	11			

There are 5 discrepancies between the modelled and reference sequences:

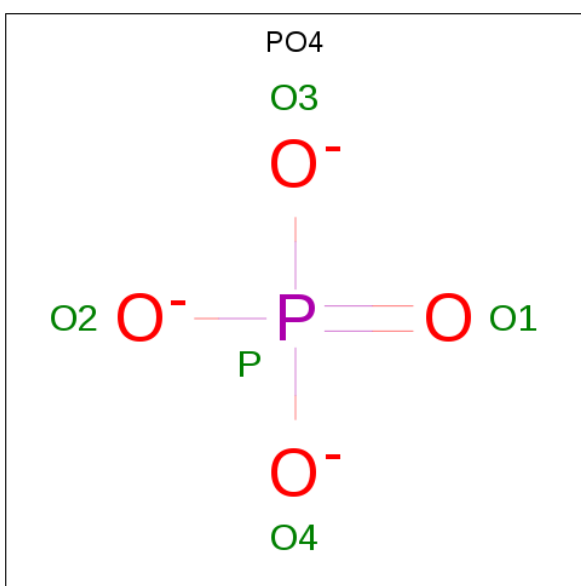
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LYS	ARG	ENGINEERED MUTATION	UNP P04818
B	163	LYS	ARG	ENGINEERED MUTATION	UNP P04818
C	163	LYS	ARG	ENGINEERED MUTATION	UNP P04818
D	163	LYS	ARG	ENGINEERED MUTATION	UNP P04818
E	163	LYS	ARG	ENGINEERED MUTATION	UNP P04818

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 20	C 10	N 3	O 6	S 1	0	0
2	D	1	Total 20	C 10	N 3	O 6	S 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	C	1	Total O P 5 4 1	0	0

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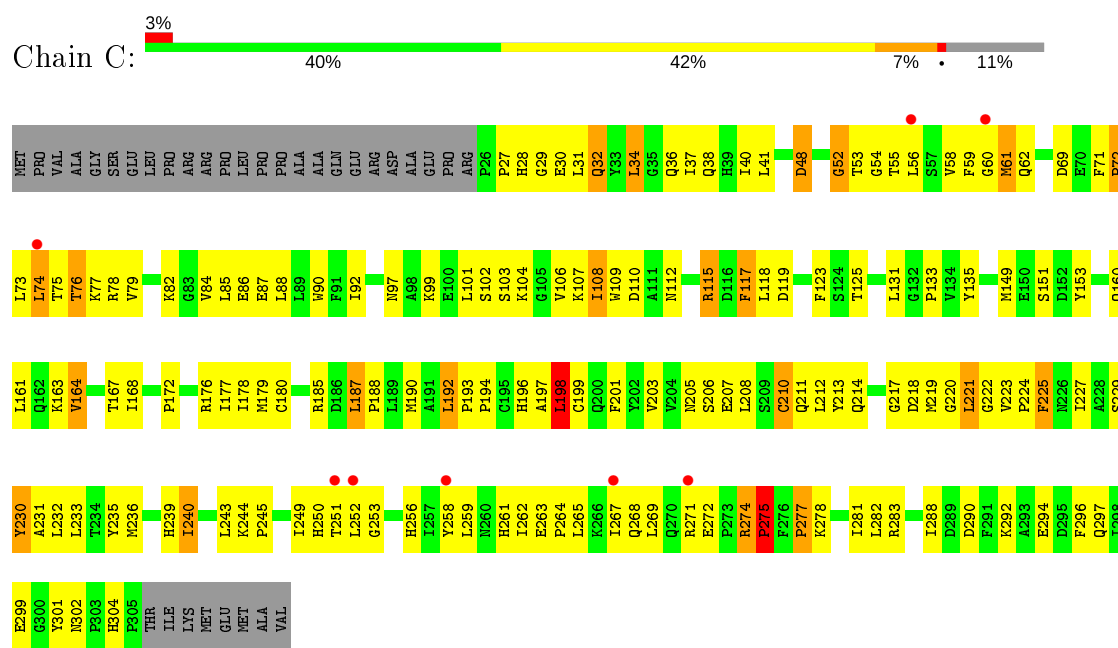
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		

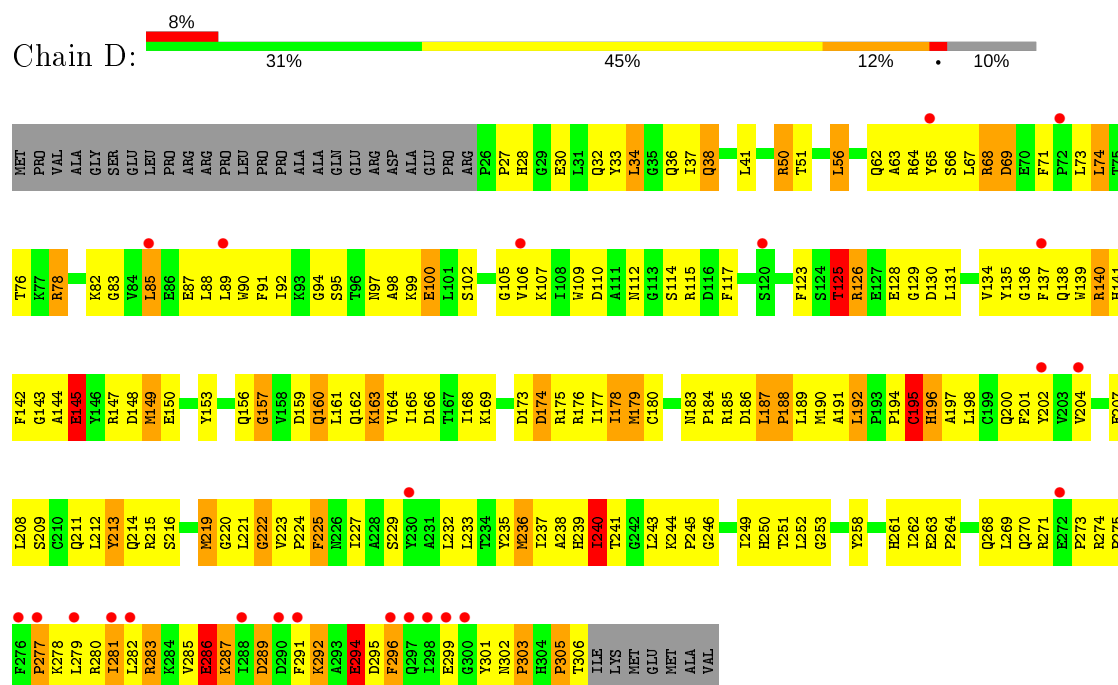
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	12	Total	O	0	0
			12	12		
4	C	12	Total	O	0	0
			12	12		
4	D	8	Total	O	0	0
			8	8		
4	E	16	Total	O	0	0
			16	16		

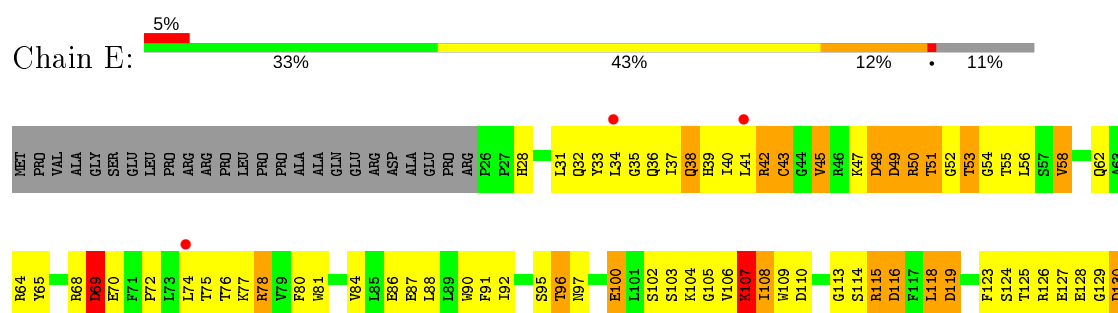




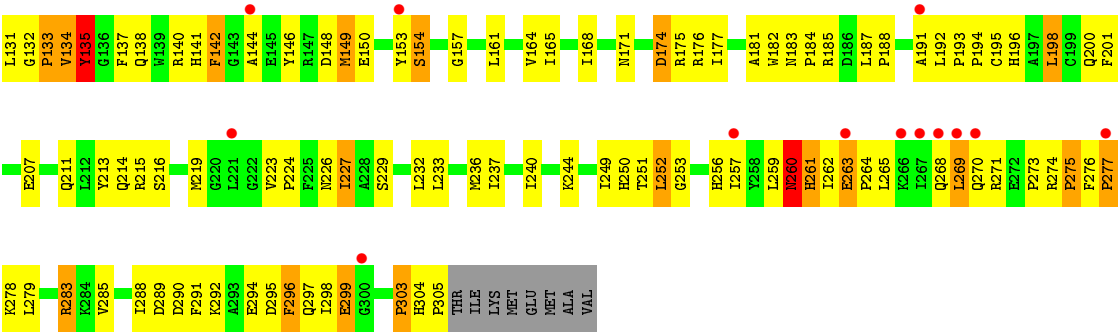
• Molecule 1: Thymidylate synthase



• Molecule 1: Thymidylate synthase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	201.80 Å   123.11 Å   99.93 Å 90.00°   115.75°   90.00°	Depositor
Resolution (Å)	45.46 – 2.75 49.86 – 2.75	Depositor EDS
% Data completeness (in resolution range)	78.7 (45.46-2.75) 82.5 (49.86-2.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.73 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.234   ,   0.293 0.240   ,   0.234	Depositor DCC
$R_{free}$ test set	5126 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.4	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.73% 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: GSH, PO4

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	0.47	0/2328	0.70	0/3150
1	B	0.39	0/2328	0.66	0/3150
1	C	0.41	0/2321	0.69	1/3140 (0.0%)
1	D	0.38	0/2328	0.71	3/3150 (0.1%)
1	E	0.37	0/2321	0.67	0/3140
All	All	0.40	0/11626	0.69	4/15730 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	2
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	HIS	N-CA-C	-8.40	88.32	111.00
1	D	34	LEU	N-CA-C	-5.60	95.88	111.00
1	D	195	CYS	O-C-N	-5.51	113.88	122.70
1	C	198	LEU	CA-CB-CG	5.08	126.98	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	230	TYR	Sidechain
1	D	195	CYS	Mainchain
1	D	213	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2268	0	2235	99	0
1	B	2268	0	2235	171	0
1	C	2261	0	2228	158	0
1	D	2268	0	2234	235	0
1	E	2261	0	2228	233	0
2	A	20	0	15	0	0
2	D	20	0	12	10	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
4	A	16	0	0	1	0
4	B	12	0	0	1	0
4	C	12	0	0	0	0
4	D	8	0	0	3	0
4	E	16	0	0	1	0
All	All	11445	0	11187	862	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 38.

All (862) 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:D:281:ILE:H	1:D:281:ILE:HD13	1.17	1.04
1:D:177:ILE:HG21	1:D:201:PHE:HB2	1.37	1.03
1:E:263:GLU:HG2	1:E:264:PRO:HD3	1.32	1.03
1:E:118:LEU:HD12	1:E:118:LEU:H	1.24	1.00
1:E:50:ARG:HH11	1:E:50:ARG:HB3	1.27	0.95
1:D:68:ARG:HD2	1:D:246:GLY:HA2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:HG22	1:A:177:ILE:HG22	1.54	0.89
1:D:176:ARG:HD3	1:E:193:PRO:HG2	1.54	0.88
1:D:32:GLN:HE21	1:D:64:ARG:H	1.22	0.88
1:D:78:ARG:HH11	1:D:78:ARG:HB2	1.37	0.88
1:B:192:LEU:H	1:B:192:LEU:HD23	1.36	0.87
1:D:238:ALA:HB3	4:D:322:HOH:O	1.74	0.87
1:D:50:ARG:HH21	1:D:50:ARG:HB3	1.38	0.87
1:B:281:ILE:HD12	1:B:281:ILE:H	1.38	0.86
1:D:222:GLY:HA3	2:D:314:GSH:HA32	1.57	0.86
1:B:185:ARG:HH11	1:B:185:ARG:HG3	1.42	0.85
1:C:172:PRO:HB3	1:C:203:VAL:HG11	1.57	0.85
1:D:164:VAL:O	1:D:168:ILE:HG13	1.77	0.84
1:D:160:GLN:O	1:D:164:VAL:HG23	1.79	0.83
1:D:123:PHE:HZ	1:D:189:LEU:HA	1.44	0.83
1:D:82:LYS:NZ	1:D:105:GLY:HA3	1.93	0.82
1:D:74:LEU:HG	1:D:224:PRO:HB3	1.59	0.82
1:C:223:VAL:O	1:C:227:ILE:HG13	1.80	0.81
1:D:62:GLN:HA	1:D:250:HIS:O	1.81	0.81
1:B:74:LEU:HD12	1:B:224:PRO:HB3	1.61	0.81
1:E:135:TYR:HD2	1:E:135:TYR:H	1.29	0.81
1:E:70:GLU:HA	1:E:278:LYS:HG2	1.63	0.80
1:A:274:ARG:HD2	1:A:302:ASN:O	1.82	0.80
1:C:74:LEU:HD12	1:C:224:PRO:HB3	1.61	0.80
1:D:85:LEU:HD22	1:D:232:LEU:HD21	1.64	0.80
1:D:82:LYS:HZ3	1:D:105:GLY:HA3	1.47	0.79
1:B:280:ARG:HD3	1:B:299:GLU:OE1	1.83	0.79
1:E:113:GLY:O	1:E:118:LEU:HD11	1.81	0.79
1:C:73:LEU:HD11	1:C:79:VAL:HB	1.63	0.79
1:D:239:HIS:ND1	1:D:281:ILE:HG13	1.98	0.79
1:E:35:GLY:HA2	1:E:38:GLN:HE21	1.48	0.79
1:B:90:TRP:HB2	1:B:101:LEU:HD23	1.64	0.79
1:D:78:ARG:HH12	1:D:303:PRO:HG2	1.46	0.79
1:C:109:TRP:CZ3	1:C:192:LEU:HD11	2.19	0.78
1:E:185:ARG:O	1:E:188:PRO:HD2	1.83	0.78
1:E:37:ILE:HD11	1:E:219:MET:HB3	1.66	0.78
1:E:74:LEU:HD12	1:E:224:PRO:HB3	1.66	0.78
1:E:37:ILE:HD13	1:E:40:ILE:HD12	1.64	0.77
1:B:88:LEU:O	1:B:92:ILE:HG13	1.84	0.77
1:D:274:ARG:HB3	1:D:275:PRO:HD2	1.66	0.77
1:E:78:ARG:HG3	1:E:78:ARG:HH11	1.49	0.77
1:C:180:CYS:SG	1:C:198:LEU:HD23	2.25	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:GLN:HB3	1:D:252:LEU:HD23	1.67	0.76
1:E:268:GLN:HG3	1:E:271:ARG:HD2	1.67	0.76
1:E:77:LYS:HD3	1:E:78:ARG:H	1.47	0.76
1:D:190:MET:SD	1:D:194:PRO:HD3	2.26	0.75
1:E:62:GLN:HG3	1:E:251:THR:OG1	1.85	0.75
1:D:222:GLY:HA3	2:D:314:GSH:CA3	2.17	0.75
1:D:177:ILE:CG2	1:D:201:PHE:HB2	2.13	0.75
1:B:277:PRO:HB2	1:B:298:ILE:HG22	1.69	0.74
1:D:140:ARG:HA	1:D:159:ASP:HA	1.69	0.74
1:B:265:LEU:O	1:B:269:LEU:HB2	1.87	0.74
1:D:78:ARG:NH1	1:D:303:PRO:HG2	2.02	0.74
1:E:182:TRP:O	1:E:184:PRO:HD3	1.86	0.74
1:B:281:ILE:N	1:B:281:ILE:HD12	2.02	0.74
1:D:38:GLN:HG2	1:D:269:LEU:HD21	1.70	0.74
1:C:240:ILE:HD11	1:C:288:ILE:N	2.02	0.74
1:D:289:ASP:N	1:D:289:ASP:OD2	2.21	0.74
1:C:108:ILE:HG13	1:C:109:TRP:CD1	2.23	0.73
1:D:140:ARG:HB2	1:D:141:HIS:CE1	2.23	0.73
1:A:263:GLU:HB2	1:A:264:PRO:HD3	1.68	0.73
1:A:257:ILE:HG21	1:A:265:LEU:HD12	1.70	0.73
1:C:164:VAL:HG12	1:C:177:ILE:HG22	1.71	0.73
1:C:31:LEU:HA	1:C:34:LEU:HD12	1.71	0.73
1:C:222:GLY:H	1:C:224:PRO:HD2	1.54	0.72
1:C:263:GLU:HB2	1:C:264:PRO:HD3	1.70	0.72
1:E:279:LEU:HD11	1:E:296:PHE:HB3	1.70	0.72
1:B:282:LEU:HD12	1:B:283:ARG:N	2.04	0.72
1:C:232:LEU:HG	1:C:236:MET:HE3	1.71	0.72
1:D:123:PHE:CZ	1:D:189:LEU:HA	2.23	0.72
1:B:219:MET:SD	1:B:223:VAL:HG21	2.30	0.71
1:C:164:VAL:HG12	1:C:177:ILE:CG2	2.20	0.71
1:B:282:LEU:HD12	1:B:283:ARG:H	1.53	0.71
1:D:68:ARG:O	1:D:69:ASP:HB2	1.88	0.71
1:E:127:GLU:O	1:E:129:GLY:N	2.23	0.71
1:B:165:ILE:HG21	1:B:240:ILE:HD11	1.72	0.71
1:C:88:LEU:O	1:C:92:ILE:HG13	1.90	0.71
1:E:77:LYS:CG	1:E:78:ARG:H	2.04	0.71
1:D:76:THR:HG23	1:D:271:ARG:HB2	1.73	0.71
1:D:198:LEU:HD11	1:E:213:TYR:CD1	2.26	0.71
1:D:74:LEU:H	1:D:74:LEU:HD22	1.54	0.71
1:E:50:ARG:HH11	1:E:50:ARG:CB	2.03	0.70
1:E:195:CYS:O	1:E:214:GLN:HA	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:LYS:CD	1:E:78:ARG:H	2.05	0.70
1:C:249:ILE:HD12	1:C:249:ILE:N	2.07	0.70
1:C:41:LEU:HD23	1:C:56:LEU:HD22	1.74	0.70
1:D:32:GLN:HE21	1:D:64:ARG:N	1.90	0.70
1:D:76:THR:HG22	1:D:268:GLN:HG2	1.74	0.69
1:B:30:GLU:HG3	1:B:74:LEU:HD22	1.73	0.69
1:C:75:THR:HG21	1:C:274:ARG:O	1.91	0.69
1:D:68:ARG:HG3	1:D:245:PRO:O	1.90	0.69
1:B:279:LEU:HD11	1:B:296:PHE:HB3	1.73	0.69
1:E:132:GLY:HA2	1:E:146:TYR:CE2	2.27	0.69
1:B:285:VAL:HG11	1:B:290:ASP:HB2	1.75	0.69
1:D:281:ILE:N	1:D:281:ILE:HD13	2.02	0.69
1:E:118:LEU:CD1	1:E:118:LEU:H	2.04	0.69
1:C:281:ILE:HD12	1:C:281:ILE:O	1.93	0.69
1:D:287:LYS:HB2	1:D:287:LYS:NZ	2.08	0.68
1:C:206:SER:HA	1:C:243:LEU:HD22	1.76	0.68
1:C:196:HIS:HB2	1:C:212:LEU:HD11	1.75	0.68
1:A:102:SER:HB2	1:A:110:ASP:OD1	1.93	0.68
1:D:74:LEU:CD2	1:D:74:LEU:H	2.06	0.68
1:B:277:PRO:HB3	1:B:301:TYR:HB2	1.75	0.68
1:D:285:VAL:HG21	1:D:291:PHE:CE1	2.29	0.68
1:B:268:GLN:HA	1:B:271:ARG:HD2	1.74	0.68
1:D:130:ASP:OD1	1:D:149:MET:HB3	1.93	0.67
1:D:83:GLY:HA2	1:D:106:VAL:HG21	1.75	0.67
1:C:223:VAL:HG13	1:C:250:HIS:HE1	1.58	0.67
1:D:140:ARG:NE	1:D:161:LEU:HD23	2.10	0.67
1:E:263:GLU:CG	1:E:264:PRO:HD3	2.19	0.67
1:E:135:TYR:HE1	1:E:196:HIS:CD2	2.13	0.67
1:E:141:HIS:O	1:E:157:GLY:HA3	1.95	0.67
1:A:28:HIS:ND1	1:A:273:PRO:HB2	2.09	0.67
1:E:183:ASN:O	1:E:187:LEU:HB2	1.95	0.66
1:E:47:LYS:CG	1:E:48:ASP:H	2.08	0.66
1:A:86:GLU:HG2	1:A:104:LYS:HB2	1.77	0.66
1:A:187:LEU:HA	1:A:190:MET:HE2	1.77	0.66
1:C:196:HIS:HD2	1:C:230:TYR:OH	1.77	0.66
2:D:314:GSH:HB13	1:E:175:ARG:NH2	2.09	0.66
1:A:205:ASN:HD21	1:B:45:VAL:HG11	1.60	0.66
1:D:177:ILE:O	1:D:178:ILE:HD12	1.95	0.66
1:D:238:ALA:HB1	1:D:243:LEU:O	1.95	0.66
1:D:160:GLN:HE22	1:D:180:CYS:H	1.44	0.66
1:C:112:ASN:HA	1:C:117:PHE:CD1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ILE:HG13	1:C:109:TRP:HD1	1.59	0.66
1:E:64:ARG:NH1	1:E:249:ILE:HD11	2.11	0.65
1:D:241:THR:OG1	1:D:243:LEU:HD12	1.96	0.65
1:C:196:HIS:CB	1:C:212:LEU:HD11	2.26	0.65
1:E:135:TYR:HE1	1:E:196:HIS:HD2	1.45	0.65
1:E:96:THR:HG22	1:E:132:GLY:O	1.97	0.65
1:D:195:CYS:O	1:D:195:CYS:SG	2.55	0.65
1:E:148:ASP:C	1:E:150:GLU:H	2.00	0.65
1:B:90:TRP:CB	1:B:101:LEU:HD23	2.26	0.65
1:D:149:MET:HG2	1:D:150:GLU:N	2.10	0.65
1:E:127:GLU:H	1:E:127:GLU:CD	1.99	0.65
1:A:38:GLN:HG2	1:A:269:LEU:HD13	1.79	0.65
1:E:97:ASN:HD22	1:E:149:MET:CE	2.10	0.65
1:D:65:TYR:CE2	1:D:227:ILE:HD13	2.33	0.64
1:B:161:LEU:HA	1:B:179:MET:CE	2.27	0.64
1:E:118:LEU:HD23	1:E:126:ARG:HB2	1.77	0.64
1:E:240:ILE:HD11	1:E:288:ILE:HA	1.78	0.64
1:B:283:ARG:HG2	1:B:284:LYS:N	2.11	0.64
1:D:125:THR:HG23	1:D:126:ARG:H	1.60	0.64
1:A:184:PRO:HG2	1:B:160:GLN:NE2	2.12	0.64
1:E:213:TYR:HD2	1:E:251:THR:HG22	1.62	0.64
1:B:33:TYR:O	1:B:37:ILE:HG12	1.98	0.64
1:B:88:LEU:CD2	1:B:92:ILE:HD11	2.27	0.64
1:C:74:LEU:HD12	1:C:224:PRO:CB	2.28	0.64
1:E:97:ASN:HB2	1:E:149:MET:HE3	1.79	0.64
1:D:305:PRO:O	1:D:306:THR:HG23	1.98	0.64
1:D:32:GLN:NE2	1:D:64:ARG:H	1.92	0.64
1:C:168:ILE:HD13	1:C:208:LEU:HD11	1.80	0.64
1:D:281:ILE:H	1:D:281:ILE:CD1	1.95	0.63
1:E:37:ILE:C	1:E:39:HIS:H	2.01	0.63
1:B:72:PRO:HA	1:B:276:PHE:CE1	2.33	0.63
1:E:108:ILE:HG23	1:E:109:TRP:CD1	2.34	0.63
1:D:169:LYS:NZ	1:D:169:LYS:HB2	2.14	0.63
1:A:142:PHE:CE2	1:B:184:PRO:HD2	2.33	0.63
1:E:81:TRP:CH2	1:E:298:ILE:HD11	2.34	0.63
1:E:77:LYS:HB2	1:E:268:GLN:OE1	1.98	0.63
1:B:29:GLY:HA3	1:B:276:PHE:HE2	1.64	0.62
1:E:55:THR:O	1:E:56:LEU:HD12	1.99	0.62
1:B:147:ARG:HH21	1:B:151:SER:HB2	1.64	0.62
1:E:33:TYR:O	1:E:36:GLN:HB3	1.99	0.62
1:B:80:PHE:HE2	1:B:106:VAL:HG13	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:TYR:HA	1:B:156:GLN:NE2	2.15	0.62
1:B:82:LYS:O	1:B:86:GLU:HB2	1.98	0.62
1:B:87:GLU:HA	1:B:101:LEU:HD21	1.82	0.62
1:E:49:ASP:CG	1:E:53:THR:HG22	2.19	0.62
1:B:161:LEU:HA	1:B:179:MET:HE1	1.82	0.62
1:D:282:LEU:HD22	1:D:282:LEU:H	1.65	0.61
1:D:50:ARG:HB3	1:D:50:ARG:NH2	2.13	0.61
1:D:89:LEU:HD23	1:D:89:LEU:O	2.00	0.61
1:C:294:GLU:H	1:C:294:GLU:CD	2.02	0.61
1:D:32:GLN:HB3	1:D:65:TYR:CE1	2.36	0.61
1:D:32:GLN:HB3	1:D:65:TYR:HE1	1.64	0.61
1:E:75:THR:HG21	1:E:274:ARG:O	2.01	0.61
1:D:99:LYS:HD2	1:D:128:GLU:O	2.01	0.61
1:D:50:ARG:HD2	2:D:314:GSH:O12	2.00	0.61
1:D:200:GLN:HE22	1:E:253:GLY:HA3	1.66	0.61
1:D:250:HIS:HD2	4:D:319:HOH:O	1.84	0.61
1:D:33:TYR:HB2	1:D:65:TYR:OH	2.00	0.61
1:E:118:LEU:HD23	1:E:126:ARG:CB	2.31	0.60
1:B:281:ILE:CD1	1:B:281:ILE:H	2.13	0.60
1:C:41:LEU:HA	1:C:56:LEU:CD2	2.32	0.60
1:D:140:ARG:HH11	1:D:140:ARG:HG3	1.66	0.60
1:D:253:GLY:HA3	1:E:200:GLN:HE22	1.66	0.60
1:E:132:GLY:O	1:E:134:VAL:HG22	2.01	0.60
1:E:35:GLY:HA2	1:E:38:GLN:HG2	1.83	0.60
1:D:88:LEU:O	1:D:92:ILE:HG13	2.02	0.60
1:E:223:VAL:O	1:E:227:ILE:HG12	2.01	0.60
1:B:109:TRP:CZ3	1:B:192:LEU:HD21	2.36	0.60
1:C:201:PHE:CD1	1:C:210:CYS:HB2	2.36	0.60
1:D:214:GLN:HB3	1:D:252:LEU:CD2	2.30	0.60
1:D:91:PHE:O	1:D:94:GLY:N	2.34	0.60
1:A:148:ASP:OD2	1:A:151:SER:N	2.35	0.60
1:C:164:VAL:O	1:C:168:ILE:HG13	2.02	0.60
1:B:223:VAL:HB	1:B:224:PRO:HD3	1.84	0.59
1:B:262:ILE:O	1:B:266:LYS:HD3	2.00	0.59
1:B:72:PRO:HA	1:B:276:PHE:CD1	2.37	0.59
1:B:30:GLU:OE1	1:B:76:THR:HG23	2.02	0.59
1:C:34:LEU:HD21	1:C:76:THR:HG21	1.84	0.59
1:D:142:PHE:CE2	1:E:184:PRO:HD2	2.37	0.59
1:D:222:GLY:CA	2:D:314:GSH:HA32	2.29	0.59
1:B:192:LEU:N	1:B:192:LEU:HD23	2.13	0.59
1:D:221:LEU:HD11	1:D:261:HIS:HE1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:SER:HA	1:E:106:VAL:O	2.02	0.59
1:E:140:ARG:NH2	1:E:161:LEU:HD23	2.17	0.59
1:D:173:ASP:N	1:D:173:ASP:OD1	2.35	0.59
1:E:127:GLU:CD	1:E:127:GLU:N	2.54	0.59
1:A:285:VAL:HG21	1:A:291:PHE:CD1	2.38	0.59
1:D:291:PHE:O	1:D:292:LYS:HE3	2.02	0.59
1:B:249:ILE:HD13	1:B:249:ILE:N	2.16	0.59
1:D:153:TYR:HA	1:D:156:GLN:NE2	2.18	0.59
1:E:133:PRO:HG3	1:E:146:TYR:CG	2.38	0.59
1:C:222:GLY:N	1:C:224:PRO:HD2	2.16	0.59
1:C:261:HIS:O	1:C:265:LEU:HG	2.02	0.59
1:C:264:PRO:O	1:C:267:ILE:HB	2.03	0.59
1:C:53:THR:HG22	1:C:54:GLY:N	2.18	0.59
1:D:280:ARG:O	1:D:296:PHE:HA	2.03	0.59
1:D:83:GLY:HA2	1:D:106:VAL:CG2	2.32	0.59
1:B:301:TYR:O	1:B:303:PRO:HD3	2.03	0.59
1:C:86:GLU:OE2	1:C:104:LYS:NZ	2.36	0.59
1:B:218:ASP:OD1	1:B:221:LEU:HB2	2.03	0.59
1:B:285:VAL:HG12	1:B:286:GLU:N	2.17	0.59
1:E:187:LEU:H	1:E:188:PRO:HD2	1.67	0.59
1:E:32:GLN:O	1:E:36:GLN:HB2	2.03	0.58
1:B:74:LEU:HD12	1:B:224:PRO:CB	2.31	0.58
1:D:197:ALA:HB1	1:E:198:LEU:HD21	1.85	0.58
1:A:176:ARG:HD3	1:B:193:PRO:HG3	1.84	0.58
1:C:38:GLN:HG3	1:C:269:LEU:HD13	1.86	0.58
1:D:76:THR:CG2	1:D:268:GLN:HG2	2.32	0.58
1:D:76:THR:HG21	1:D:268:GLN:O	2.02	0.58
1:B:185:ARG:NH1	1:B:185:ARG:HG3	2.16	0.58
1:C:223:VAL:N	1:C:224:PRO:HD2	2.17	0.58
1:D:62:GLN:NE2	1:D:211:GLN:HE22	2.01	0.58
1:E:64:ARG:CZ	1:E:249:ILE:HD11	2.33	0.58
1:B:87:GLU:O	1:B:90:TRP:HB3	2.03	0.58
1:E:182:TRP:O	1:E:182:TRP:CD1	2.57	0.58
1:A:187:LEU:HB2	1:A:188:PRO:CD	2.34	0.58
1:D:235:TYR:C	1:D:237:ILE:H	2.06	0.58
1:D:279:LEU:HD11	1:D:296:PHE:HB3	1.86	0.58
1:D:30:GLU:OE1	1:D:74:LEU:HA	2.04	0.58
1:E:31:LEU:HD23	1:E:273:PRO:HG2	1.86	0.58
1:B:77:LYS:O	1:B:77:LYS:HD3	2.04	0.58
1:C:115:ARG:O	1:C:115:ARG:HD3	2.04	0.58
1:A:268:GLN:O	1:A:271:ARG:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:109:TRP:CE3	1:E:131:LEU:HD13	2.39	0.57
1:B:215:ARG:HG3	1:B:216:SER:N	2.18	0.57
1:B:285:VAL:HG12	1:B:286:GLU:H	1.68	0.57
1:D:187:LEU:HD13	1:D:190:MET:HE1	1.85	0.57
1:E:261:HIS:CD2	1:E:261:HIS:N	2.72	0.57
1:E:87:GLU:O	1:E:90:TRP:HB3	2.04	0.57
1:B:192:LEU:H	1:B:192:LEU:CD2	2.13	0.57
1:E:107:LYS:HE2	1:E:107:LYS:H	1.70	0.57
1:A:88:LEU:HD23	1:A:236:MET:CE	2.34	0.57
1:D:223:VAL:HB	1:D:224:PRO:HD3	1.87	0.57
1:B:168:ILE:HD13	1:B:208:LEU:HD11	1.87	0.57
1:B:101:LEU:O	1:B:101:LEU:HD13	2.05	0.57
1:C:221:LEU:HG	1:C:221:LEU:O	2.05	0.57
1:D:102:SER:HB3	1:D:110:ASP:OD2	2.04	0.57
1:D:74:LEU:CG	1:D:224:PRO:HB3	2.34	0.57
1:A:305:PRO:O	1:A:306:THR:HB	2.05	0.56
1:C:84:VAL:HG22	1:C:225:PHE:CD2	2.40	0.56
1:D:198:LEU:HD12	1:D:198:LEU:C	2.25	0.56
1:E:118:LEU:N	1:E:118:LEU:HD12	2.08	0.56
1:B:117:PHE:O	1:B:120:SER:HB3	2.05	0.56
1:D:176:ARG:HD3	1:E:193:PRO:CG	2.33	0.56
1:D:74:LEU:N	1:D:74:LEU:HD22	2.20	0.56
1:A:38:GLN:CG	1:A:269:LEU:HD13	2.36	0.56
1:E:252:LEU:H	1:E:252:LEU:HD12	1.70	0.56
1:E:97:ASN:HB2	1:E:149:MET:SD	2.45	0.56
1:B:90:TRP:CD1	1:B:95:SER:HB3	2.40	0.56
1:E:108:ILE:HG23	1:E:109:TRP:HD1	1.70	0.56
1:E:259:LEU:HG	1:E:262:ILE:HD11	1.87	0.56
1:A:28:HIS:ND1	1:A:273:PRO:CB	2.68	0.56
1:A:102:SER:HA	1:A:106:VAL:O	2.05	0.56
1:B:32:GLN:HE21	1:B:64:ARG:H	1.53	0.56
1:C:225:PHE:HD2	1:C:225:PHE:O	1.89	0.56
1:C:297:GLN:NE2	1:C:299:GLU:HB3	2.20	0.56
1:C:97:ASN:ND2	1:C:149:MET:SD	2.79	0.56
1:B:264:PRO:O	1:B:267:ILE:HG12	2.05	0.56
1:E:75:THR:O	1:E:303:PRO:HA	2.06	0.56
1:E:35:GLY:HA2	1:E:38:GLN:NE2	2.20	0.56
1:A:184:PRO:CG	1:B:160:GLN:HE21	2.19	0.55
1:D:107:LYS:HB3	1:D:110:ASP:OD1	2.07	0.55
1:E:268:GLN:C	1:E:270:GLN:H	2.08	0.55
1:B:84:VAL:HG13	1:B:229:SER:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ILE:HD12	1:B:219:MET:HG3	1.88	0.55
1:E:213:TYR:CD2	1:E:251:THR:HG22	2.40	0.55
1:E:80:PHE:HE2	1:E:106:VAL:HG13	1.70	0.55
1:C:192:LEU:HD22	1:C:192:LEU:O	2.07	0.55
1:E:76:THR:O	1:E:271:ARG:HD3	2.06	0.55
1:C:32:GLN:O	1:C:36:GLN:HG3	2.06	0.55
1:E:97:ASN:HB2	1:E:149:MET:CE	2.37	0.55
1:C:28:HIS:CD2	1:C:30:GLU:HB3	2.41	0.55
1:D:149:MET:HG2	1:D:150:GLU:H	1.69	0.55
1:A:40:ILE:HD12	1:A:219:MET:HG3	1.88	0.55
1:B:247:ASP:HB3	4:B:318:HOH:O	2.05	0.55
1:A:198:LEU:C	1:A:198:LEU:HD12	2.27	0.55
1:E:198:LEU:HD12	1:E:198:LEU:C	2.26	0.55
1:E:240:ILE:HD11	1:E:291:PHE:HE2	1.72	0.55
1:E:41:LEU:HA	1:E:56:LEU:HD23	1.88	0.55
1:D:240:ILE:HD12	1:D:291:PHE:HE2	1.72	0.54
1:D:34:LEU:HD22	1:D:269:LEU:HD12	1.89	0.54
1:D:177:ILE:O	1:D:200:GLN:HA	2.07	0.54
1:E:88:LEU:O	1:E:92:ILE:HG13	2.06	0.54
1:C:211:GLN:NE2	1:C:251:THR:OG1	2.39	0.54
1:D:169:LYS:HZ2	1:D:169:LYS:HB2	1.72	0.54
1:E:102:SER:O	1:E:105:GLY:N	2.38	0.54
1:A:164:VAL:HG22	1:A:177:ILE:CG2	2.33	0.54
1:A:221:LEU:HD22	1:A:221:LEU:N	2.23	0.54
1:B:115:ARG:HD3	1:B:115:ARG:O	2.08	0.54
1:E:252:LEU:N	1:E:252:LEU:HD12	2.22	0.54
1:A:271:ARG:HE	1:A:304:HIS:HB3	1.72	0.54
1:A:288:ILE:HG22	4:A:315:HOH:O	2.08	0.54
1:B:109:TRP:CE3	1:B:131:LEU:HD13	2.42	0.54
1:B:109:TRP:CH2	1:B:192:LEU:HD21	2.42	0.54
1:D:135:TYR:O	1:D:139:TRP:CD1	2.60	0.54
1:D:62:GLN:HE21	1:D:211:GLN:HE22	1.55	0.54
1:D:67:LEU:HD23	1:D:235:TYR:HE2	1.73	0.54
1:D:85:LEU:HD22	1:D:232:LEU:CD2	2.36	0.54
1:C:249:ILE:N	1:C:249:ILE:CD1	2.71	0.54
1:D:62:GLN:HE21	1:D:211:GLN:NE2	2.06	0.54
1:A:240:ILE:CG2	1:D:51:THR:HG23	2.37	0.54
1:B:59:PHE:HA	1:B:253:GLY:O	2.08	0.54
1:B:85:LEU:HD12	1:B:85:LEU:O	2.06	0.54
1:D:67:LEU:HD23	1:D:235:TYR:CE2	2.43	0.54
1:E:86:GLU:O	1:E:90:TRP:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LYS:CB	1:C:110:ASP:OD2	2.55	0.54
1:C:168:ILE:HG23	1:C:203:VAL:HG21	1.90	0.54
1:B:101:LEU:HD13	1:B:106:VAL:HB	1.89	0.54
1:E:261:HIS:O	1:E:264:PRO:HD2	2.08	0.54
1:C:192:LEU:HD13	1:C:192:LEU:H	1.73	0.53
1:D:76:THR:HG22	1:D:268:GLN:CG	2.36	0.53
1:E:299:GLU:HG3	1:E:299:GLU:O	2.09	0.53
1:B:182:TRP:CZ2	1:B:187:LEU:HD21	2.42	0.53
1:B:236:MET:O	1:B:240:ILE:HG23	2.08	0.53
1:B:88:LEU:HA	1:B:91:PHE:CD2	2.43	0.53
1:A:286:GLU:OE2	1:D:50:ARG:NH2	2.42	0.53
1:C:264:PRO:HA	1:C:267:ILE:HD12	1.90	0.53
1:A:190:MET:HE1	1:A:194:PRO:HD3	1.89	0.53
1:A:233:LEU:HD11	1:A:237:ILE:HD11	1.91	0.53
1:B:46:ARG:NH1	1:B:48:ASP:OD2	2.41	0.53
1:E:77:LYS:CG	1:E:78:ARG:N	2.72	0.53
1:C:217:GLY:HA3	1:C:252:LEU:CD2	2.38	0.53
1:D:28:HIS:CD2	1:D:273:PRO:HB2	2.43	0.53
1:D:281:ILE:HG12	1:D:281:ILE:O	2.09	0.53
1:D:175:ARG:O	1:E:215:ARG:HD2	2.07	0.53
1:C:240:ILE:CD1	1:C:288:ILE:N	2.72	0.53
1:D:174:ASP:O	1:D:177:ILE:HG12	2.09	0.53
1:E:127:GLU:C	1:E:129:GLY:H	2.11	0.53
1:E:130:ASP:HB2	1:E:149:MET:HG2	1.89	0.53
1:E:50:ARG:O	1:E:51:THR:HG23	2.08	0.53
1:E:84:VAL:HG13	1:E:229:SER:HA	1.90	0.53
1:D:250:HIS:HA	4:D:319:HOH:O	2.09	0.53
1:C:187:LEU:HA	1:C:190:MET:HG3	1.91	0.53
1:E:259:LEU:O	1:E:262:ILE:HG13	2.09	0.53
1:C:223:VAL:N	1:C:224:PRO:CD	2.72	0.52
1:D:213:TYR:CE2	1:E:211:GLN:OE1	2.62	0.52
1:E:90:TRP:CD1	1:E:95:SER:HB3	2.45	0.52
1:A:257:ILE:HG21	1:A:265:LEU:CD1	2.38	0.52
1:C:172:PRO:O	1:C:203:VAL:HB	2.10	0.52
1:D:274:ARG:HD2	1:D:302:ASN:O	2.08	0.52
1:E:292:LYS:HB2	1:E:295:ASP:OD1	2.08	0.52
1:A:232:LEU:HG	1:A:236:MET:HE3	1.90	0.52
1:A:88:LEU:HD23	1:A:236:MET:HE3	1.91	0.52
1:C:222:GLY:C	1:C:224:PRO:HD2	2.29	0.52
1:C:41:LEU:HD23	1:C:56:LEU:CD2	2.40	0.52
1:D:212:LEU:HG	1:D:213:TYR:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:TYR:HE2	1:E:211:GLN:OE1	1.92	0.52
1:E:265:LEU:O	1:E:269:LEU:N	2.40	0.52
1:D:183:ASN:HB3	1:D:186:ASP:HB2	1.90	0.52
1:B:108:ILE:HD11	1:B:109:TRP:HD1	1.74	0.52
1:C:75:THR:C	1:C:77:LYS:H	2.12	0.52
1:A:45:VAL:HG21	1:B:205:ASN:HD21	1.74	0.52
1:E:304:HIS:HB3	1:E:305:PRO:HD2	1.91	0.52
1:E:47:LYS:CG	1:E:48:ASP:N	2.73	0.52
1:B:165:ILE:HG23	1:B:241:THR:CG2	2.40	0.52
1:B:280:ARG:CD	1:B:299:GLU:OE1	2.56	0.52
1:D:178:ILE:CD1	1:D:200:GLN:HG3	2.40	0.52
1:D:294:GLU:H	1:D:294:GLU:CD	2.12	0.52
1:D:294:GLU:CD	1:D:294:GLU:N	2.63	0.52
1:B:33:TYR:CE2	1:B:224:PRO:HG3	2.45	0.52
1:A:214:GLN:HE21	1:A:217:GLY:CA	2.23	0.52
1:E:138:GLN:O	1:E:142:PHE:HB2	2.10	0.52
1:E:181:ALA:O	1:E:194:PRO:HG2	2.09	0.52
1:A:223:VAL:HB	1:A:224:PRO:HD3	1.92	0.52
1:B:118:LEU:H	1:B:118:LEU:HD12	1.75	0.52
1:E:38:GLN:HB3	1:E:269:LEU:HD21	1.91	0.52
1:B:283:ARG:HD3	1:B:295:ASP:OD1	2.10	0.51
1:B:304:HIS:ND1	1:B:305:PRO:HD2	2.26	0.51
1:C:31:LEU:HA	1:C:34:LEU:CD1	2.38	0.51
1:A:282:LEU:HD12	1:A:294:GLU:O	2.10	0.51
1:C:85:LEU:HD11	1:C:296:PHE:CD1	2.45	0.51
1:D:78:ARG:CB	1:D:78:ARG:HH11	2.17	0.51
1:B:168:ILE:HD13	1:B:208:LEU:CD1	2.40	0.51
1:B:222:GLY:O	1:B:225:PHE:N	2.42	0.51
1:C:38:GLN:HG3	1:C:269:LEU:CD1	2.40	0.51
1:C:58:VAL:HG12	1:C:59:PHE:N	2.25	0.51
1:D:261:HIS:O	1:D:264:PRO:HG2	2.09	0.51
1:E:240:ILE:CD1	1:E:288:ILE:HA	2.38	0.51
1:E:78:ARG:NH1	1:E:78:ARG:HG3	2.21	0.51
1:B:112:ASN:HD22	1:B:112:ASN:H	1.57	0.51
1:B:135:TYR:O	1:B:138:GLN:N	2.42	0.51
1:B:44:GLY:O	1:B:56:LEU:HD22	2.10	0.51
1:C:109:TRP:HZ3	1:C:192:LEU:HD11	1.74	0.51
1:D:239:HIS:O	1:D:240:ILE:HB	2.11	0.51
1:B:185:ARG:CG	1:B:185:ARG:HH11	2.18	0.51
1:C:271:ARG:HB3	1:C:304:HIS:ND1	2.25	0.51
1:A:87:GLU:O	1:A:90:TRP:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ASN:HD22	1:B:100:GLU:HB2	1.76	0.51
1:C:107:LYS:HB3	1:C:110:ASP:OD2	2.11	0.51
2:D:314:GSH:HB13	1:E:175:ARG:HH21	1.76	0.51
1:D:66:SER:C	1:D:67:LEU:HD12	2.30	0.51
1:E:49:ASP:HB3	1:E:52:GLY:CA	2.41	0.51
1:B:80:PHE:CE2	1:B:106:VAL:HG13	2.46	0.51
1:B:279:LEU:CD1	1:B:296:PHE:HB3	2.40	0.51
1:C:102:SER:HB2	1:C:110:ASP:OD1	2.11	0.50
1:E:119:ASP:HA	1:E:124:SER:OG	2.11	0.50
1:E:40:ILE:HA	1:E:58:VAL:HG21	1.93	0.50
1:D:240:ILE:HD11	1:D:287:LYS:C	2.32	0.50
1:E:74:LEU:CD1	1:E:224:PRO:HB3	2.39	0.50
1:B:161:LEU:CA	1:B:179:MET:HE1	2.40	0.50
1:B:259:LEU:O	1:B:262:ILE:HG13	2.11	0.50
1:C:168:ILE:O	1:C:172:PRO:HG3	2.11	0.50
1:C:187:LEU:N	1:C:188:PRO:CD	2.74	0.50
1:D:130:ASP:HB2	1:D:149:MET:SD	2.51	0.50
1:D:292:LYS:HE3	1:D:292:LYS:HA	1.94	0.50
1:E:100:GLU:O	1:E:103:SER:HB3	2.11	0.50
1:E:102:SER:HB3	1:E:110:ASP:OD1	2.11	0.50
1:E:164:VAL:O	1:E:168:ILE:HG13	2.11	0.50
1:C:151:SER:HB2	1:C:153:TYR:CZ	2.47	0.50
1:E:141:HIS:O	1:E:142:PHE:C	2.50	0.50
1:A:79:VAL:O	1:A:81:TRP:N	2.44	0.50
1:B:97:ASN:ND2	1:B:100:GLU:H	2.10	0.50
1:B:53:THR:HG22	1:B:53:THR:O	2.11	0.50
1:D:147:ARG:HB2	1:D:153:TYR:OH	2.11	0.50
1:E:137:PHE:CZ	1:E:144:ALA:HB3	2.46	0.50
1:E:182:TRP:CD1	1:E:184:PRO:HG3	2.47	0.50
1:E:261:HIS:C	1:E:264:PRO:HD2	2.31	0.50
1:E:263:GLU:CD	1:E:263:GLU:H	2.12	0.50
1:B:135:TYR:O	1:B:136:GLY:C	2.50	0.50
1:C:282:LEU:HD12	1:C:294:GLU:O	2.12	0.50
1:A:201:PHE:CE1	1:A:210:CYS:HB2	2.47	0.50
1:D:88:LEU:HD22	1:D:232:LEU:HD23	1.94	0.50
1:E:77:LYS:HG2	1:E:78:ARG:H	1.76	0.50
1:A:202:TYR:CE1	1:B:47:LYS:HE3	2.46	0.49
1:B:165:ILE:HD13	1:B:240:ILE:HD11	1.94	0.49
1:C:60:GLY:O	1:C:61:MET:HG2	2.11	0.49
1:A:70:GLU:HG2	1:A:276:PHE:HB2	1.93	0.49
1:D:140:ARG:HG3	1:D:140:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:LEU:HD12	1:C:188:PRO:HD3	1.92	0.49
1:C:87:GLU:O	1:C:90:TRP:HB3	2.13	0.49
1:D:225:PHE:O	1:D:229:SER:HB2	2.12	0.49
1:E:191:ALA:O	1:E:192:LEU:HB2	2.11	0.49
1:C:214:GLN:HE21	1:C:217:GLY:HA2	1.76	0.49
1:E:133:PRO:HG3	1:E:146:TYR:CB	2.43	0.49
1:E:108:ILE:HG23	1:E:109:TRP:N	2.27	0.49
1:D:187:LEU:HB2	1:D:188:PRO:HD3	1.95	0.49
1:D:190:MET:C	1:D:192:LEU:H	2.16	0.49
1:E:92:ILE:CD1	1:E:236:MET:HE1	2.43	0.49
1:E:41:LEU:HD23	1:E:56:LEU:HD22	1.94	0.49
1:C:172:PRO:HB3	1:C:203:VAL:CG1	2.35	0.49
1:D:278:LYS:HE2	1:D:280:ARG:HD2	1.94	0.49
1:C:29:GLY:O	1:C:32:GLN:HB2	2.13	0.49
1:C:235:TYR:CD1	1:C:245:PRO:HG2	2.48	0.49
1:C:259:LEU:O	1:C:262:ILE:HG13	2.13	0.49
1:D:88:LEU:HD22	1:D:232:LEU:HB3	1.94	0.49
1:E:38:GLN:HB3	1:E:269:LEU:HD11	1.94	0.49
1:A:184:PRO:HD2	1:B:142:PHE:CZ	2.48	0.49
1:A:184:PRO:CG	1:B:160:GLN:NE2	2.76	0.49
1:E:223:VAL:HB	1:E:224:PRO:HD3	1.95	0.49
1:A:126:ARG:HD3	1:A:130:ASP:HB3	1.95	0.48
1:B:259:LEU:HD12	1:B:262:ILE:HD11	1.95	0.48
1:A:170:THR:HG22	1:D:258:TYR:CD1	2.48	0.48
1:B:98:ALA:HB2	1:B:131:LEU:HD11	1.95	0.48
1:B:277:PRO:CB	1:B:298:ILE:HG22	2.41	0.48
1:C:160:GLN:O	1:C:163:LYS:HB3	2.13	0.48
1:C:207:GLU:HA	1:C:244:LYS:O	2.13	0.48
1:D:190:MET:SD	1:D:194:PRO:CD	3.00	0.48
1:E:127:GLU:HB3	4:E:327:HOH:O	2.11	0.48
1:B:168:ILE:O	1:B:172:PRO:HG3	2.12	0.48
1:C:90:TRP:HB2	1:C:101:LEU:HD13	1.95	0.48
1:E:215:ARG:HG3	1:E:216:SER:N	2.27	0.48
1:B:263:GLU:OE2	1:B:266:LYS:HE3	2.13	0.48
1:B:87:GLU:OE2	1:B:225:PHE:HE2	1.96	0.48
1:B:88:LEU:HD22	1:B:92:ILE:HD11	1.95	0.48
1:C:117:PHE:O	1:C:117:PHE:HD2	1.97	0.48
1:C:206:SER:O	1:C:243:LEU:HB3	2.13	0.48
1:B:153:TYR:O	1:B:156:GLN:HB2	2.14	0.48
1:B:260:ASN:O	1:B:262:ILE:N	2.46	0.48
1:C:118:LEU:O	1:C:123:PHE:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:TYR:O	1:E:154:SER:C	2.51	0.48
1:A:33:TYR:CE1	1:A:74:LEU:HD13	2.48	0.48
1:E:269:LEU:O	1:E:269:LEU:HG	2.14	0.48
1:B:126:ARG:NH2	1:B:126:ARG:HG3	2.28	0.48
1:D:109:TRP:CE3	1:D:131:LEU:HD13	2.48	0.48
1:D:187:LEU:O	1:D:189:LEU:N	2.46	0.48
1:D:301:TYR:O	1:D:303:PRO:HD3	2.14	0.48
1:A:169:LYS:HG3	1:A:241:THR:HG22	1.94	0.48
1:A:37:ILE:HB	1:A:269:LEU:HD21	1.96	0.48
1:B:40:ILE:CD1	1:B:219:MET:HG3	2.43	0.48
1:B:79:VAL:O	1:B:81:TRP:N	2.46	0.48
1:C:59:PHE:HA	1:C:253:GLY:O	2.14	0.48
1:E:49:ASP:HB3	1:E:52:GLY:H	1.78	0.48
1:E:62:GLN:HG3	1:E:251:THR:HG1	1.79	0.48
1:D:82:LYS:HZ1	1:D:105:GLY:HA3	1.74	0.47
1:A:192:LEU:HD13	1:A:192:LEU:N	2.29	0.47
1:A:73:LEU:HG	1:A:301:TYR:CE1	2.49	0.47
1:A:68:ARG:C	1:A:70:GLU:H	2.18	0.47
1:C:263:GLU:O	1:C:267:ILE:HG13	2.14	0.47
1:D:187:LEU:CB	1:D:188:PRO:HD3	2.44	0.47
1:E:65:TYR:CE2	1:E:227:ILE:HD12	2.50	0.47
1:A:190:MET:CE	1:A:194:PRO:HD3	2.45	0.47
1:D:239:HIS:O	1:D:239:HIS:CD2	2.67	0.47
1:C:197:ALA:O	1:C:198:LEU:HB2	2.13	0.47
1:D:183:ASN:OD1	1:D:185:ARG:HG2	2.14	0.47
1:D:280:ARG:HD3	1:D:299:GLU:OE1	2.15	0.47
1:A:261:HIS:O	1:A:264:PRO:HD2	2.15	0.47
1:B:118:LEU:N	1:B:118:LEU:HD12	2.28	0.47
1:C:74:LEU:CD1	1:C:224:PRO:HB3	2.39	0.47
1:E:187:LEU:N	1:E:188:PRO:HD2	2.28	0.47
1:A:164:VAL:HG12	1:A:165:ILE:N	2.29	0.47
1:B:88:LEU:O	1:B:88:LEU:HD23	2.15	0.47
1:B:97:ASN:ND2	1:B:100:GLU:N	2.63	0.47
1:C:112:ASN:HA	1:C:117:PHE:CE1	2.50	0.47
1:C:212:LEU:HG	1:C:213:TYR:N	2.30	0.47
1:D:32:GLN:CG	1:D:63:ALA:HB1	2.45	0.47
1:D:67:LEU:N	1:D:67:LEU:HD12	2.30	0.47
1:E:116:ASP:O	1:E:119:ASP:HB2	2.14	0.47
1:E:135:TYR:N	1:E:135:TYR:CD2	2.74	0.47
1:E:196:HIS:HE1	1:E:226:ASN:CG	2.18	0.47
1:A:259:LEU:O	1:A:262:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:LEU:O	1:D:198:LEU:HD12	2.14	0.47
1:D:235:TYR:C	1:D:237:ILE:N	2.68	0.47
1:E:107:LYS:O	1:E:109:TRP:N	2.47	0.47
1:B:223:VAL:O	1:B:227:ILE:HG13	2.15	0.47
1:C:84:VAL:HA	1:C:225:PHE:CE2	2.50	0.47
1:D:102:SER:HB3	1:D:110:ASP:CG	2.34	0.47
1:D:98:ALA:HB3	1:D:129:GLY:HA2	1.96	0.47
1:D:202:TYR:CD1	1:E:47:LYS:HE2	2.49	0.47
1:C:219:MET:HA	1:C:223:VAL:HG21	1.95	0.47
1:C:58:VAL:CG1	1:C:59:PHE:N	2.78	0.47
1:D:279:LEU:HD11	1:D:296:PHE:CB	2.44	0.47
1:E:132:GLY:O	1:E:134:VAL:N	2.46	0.47
1:D:76:THR:HG22	1:D:76:THR:O	2.15	0.46
1:E:259:LEU:O	1:E:261:HIS:N	2.48	0.46
1:D:221:LEU:HD11	1:D:261:HIS:CE1	2.49	0.46
1:E:42:ARG:HG2	1:E:42:ARG:HH21	1.79	0.46
1:A:205:ASN:ND2	1:B:45:VAL:HG11	2.29	0.46
1:C:75:THR:O	1:C:77:LYS:N	2.48	0.46
1:D:140:ARG:CA	1:D:159:ASP:HA	2.42	0.46
1:D:109:TRP:HB3	1:D:131:LEU:HD11	1.98	0.46
1:E:107:LYS:CE	1:E:107:LYS:H	2.27	0.46
1:A:151:SER:HB2	1:A:153:TYR:CE1	2.50	0.46
1:D:90:TRP:O	1:D:95:SER:HB3	2.16	0.46
1:E:261:HIS:HA	1:E:264:PRO:HD2	1.98	0.46
1:B:38:GLN:HG3	1:B:269:LEU:HD11	1.97	0.46
1:D:287:LYS:HZ3	1:D:287:LYS:HB2	1.80	0.46
1:E:31:LEU:CD2	1:E:273:PRO:HG2	2.45	0.46
1:B:240:ILE:HG13	1:B:240:ILE:O	2.16	0.46
1:B:294:GLU:CD	1:B:294:GLU:H	2.17	0.46
1:C:272:GLU:O	1:C:304:HIS:CE1	2.69	0.46
1:D:123:PHE:HB3	1:D:126:ARG:HD2	1.97	0.46
1:E:107:LYS:NZ	1:E:107:LYS:HB3	2.30	0.46
1:E:259:LEU:HG	1:E:262:ILE:CD1	2.46	0.46
1:E:40:ILE:O	1:E:56:LEU:HD23	2.15	0.46
1:A:112:ASN:ND2	1:A:192:LEU:HD12	2.31	0.46
1:B:89:LEU:O	1:B:93:LYS:HG3	2.16	0.46
1:D:160:GLN:NE2	1:D:180:CYS:H	2.11	0.46
1:E:215:ARG:NH1	1:E:216:SER:HB2	2.31	0.46
1:E:274:ARG:CZ	1:E:304:HIS:HE1	2.29	0.46
1:A:45:VAL:HG21	1:B:205:ASN:ND2	2.31	0.46
1:B:123:PHE:HB3	1:B:126:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:SER:OG	1:B:256:HIS:HE1	1.99	0.46
1:D:296:PHE:N	1:D:296:PHE:CD1	2.83	0.46
1:E:125:THR:O	1:E:125:THR:HG22	2.16	0.46
1:E:62:GLN:HA	1:E:250:HIS:O	2.16	0.46
1:A:107:LYS:HA	1:A:110:ASP:OD2	2.16	0.46
1:B:97:ASN:ND2	1:B:100:GLU:HB2	2.31	0.46
1:C:40:ILE:HD12	1:C:219:MET:HG3	1.98	0.46
1:D:148:ASP:N	1:D:153:TYR:OH	2.49	0.46
1:D:88:LEU:HD21	1:D:233:LEU:HD13	1.97	0.46
1:E:107:LYS:CG	1:E:108:ILE:H	2.29	0.46
1:E:171:ASN:HB3	1:E:174:ASP:HB2	1.98	0.46
1:E:193:PRO:HA	1:E:194:PRO:HD3	1.83	0.46
1:A:214:GLN:HE21	1:A:217:GLY:HA3	1.81	0.45
1:A:97:ASN:HB2	1:A:149:MET:SD	2.56	0.45
1:B:215:ARG:HG3	1:B:216:SER:H	1.81	0.45
1:B:88:LEU:HD13	1:B:232:LEU:HD23	1.97	0.45
1:E:148:ASP:C	1:E:150:GLU:N	2.67	0.45
1:C:185:ARG:O	1:C:188:PRO:HD2	2.15	0.45
1:C:78:ARG:HA	1:C:301:TYR:OH	2.16	0.45
1:C:53:THR:CG2	1:C:54:GLY:N	2.79	0.45
1:D:97:ASN:HD22	1:D:100:GLU:H	1.64	0.45
1:D:123:PHE:N	1:D:123:PHE:CD2	2.83	0.45
1:D:287:LYS:HB2	1:D:287:LYS:HZ2	1.80	0.45
1:B:128:GLU:O	1:B:128:GLU:OE1	2.34	0.45
1:B:36:GLN:O	1:B:40:ILE:HG13	2.16	0.45
1:D:163:LYS:HD3	1:D:163:LYS:O	2.17	0.45
1:E:211:GLN:HB2	1:E:249:ILE:HB	1.97	0.45
1:E:38:GLN:CB	1:E:269:LEU:HD21	2.46	0.45
1:C:37:ILE:HG23	1:C:265:LEU:HD13	1.98	0.45
1:C:53:THR:HG22	1:C:54:GLY:H	1.82	0.45
1:E:123:PHE:N	1:E:123:PHE:CD2	2.85	0.45
1:B:236:MET:HB3	1:B:236:MET:HE3	1.77	0.45
1:C:292:LYS:HB3	1:C:294:GLU:OE2	2.17	0.45
1:C:48:ASP:OD2	1:C:52:GLY:HA2	2.16	0.45
1:D:215:ARG:HG3	1:D:215:ARG:HH11	1.82	0.45
1:D:225:PHE:O	1:D:225:PHE:CD2	2.69	0.45
1:E:261:HIS:O	1:E:265:LEU:HG	2.15	0.45
1:E:47:LYS:HG3	1:E:48:ASP:H	1.77	0.45
1:C:225:PHE:C	1:C:225:PHE:CD2	2.90	0.45
1:D:198:LEU:HD11	1:E:213:TYR:CE1	2.51	0.45
1:E:37:ILE:C	1:E:39:HIS:N	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:NH2	1:A:189:LEU:O	2.37	0.45
1:C:201:PHE:CE1	1:C:210:CYS:HB2	2.51	0.45
1:D:139:TRP:HA	1:D:179:MET:CE	2.47	0.45
1:B:196:HIS:O	1:B:197:ALA:C	2.55	0.45
1:B:248:PHE:C	1:B:249:ILE:HD13	2.37	0.45
1:C:62:GLN:O	1:C:62:GLN:HG2	2.16	0.45
1:D:138:GLN:O	1:D:160:GLN:OE1	2.35	0.45
1:D:220:GLY:O	1:D:221:LEU:HD23	2.17	0.45
1:D:62:GLN:NE2	1:D:211:GLN:NE2	2.64	0.45
1:E:211:GLN:HA	1:E:249:ILE:O	2.16	0.45
1:E:72:PRO:HA	1:E:276:PHE:CE1	2.52	0.45
1:B:263:GLU:HB2	1:B:264:PRO:HD3	1.98	0.45
1:D:125:THR:O	1:D:126:ARG:O	2.34	0.45
1:D:137:PHE:HE1	1:D:153:TYR:CE2	2.34	0.45
1:D:32:GLN:HG3	1:D:63:ALA:HB1	1.98	0.45
1:B:62:GLN:NE2	1:B:211:GLN:HE22	2.15	0.45
1:D:141:HIS:O	1:D:142:PHE:C	2.55	0.45
1:D:92:ILE:C	1:D:94:GLY:N	2.70	0.45
1:E:185:ARG:C	1:E:187:LEU:H	2.19	0.45
1:E:276:PHE:HD1	1:E:277:PRO:HD2	1.82	0.45
1:E:49:ASP:HB3	1:E:52:GLY:N	2.32	0.45
1:A:59:PHE:HA	1:A:253:GLY:O	2.17	0.44
1:A:78:ARG:HG3	1:A:78:ARG:HH11	1.82	0.44
1:B:279:LEU:HA	1:B:297:GLN:O	2.16	0.44
1:C:71:PHE:HA	1:C:72:PRO:HD2	1.79	0.44
1:E:55:THR:C	1:E:56:LEU:HD12	2.37	0.44
1:E:279:LEU:CD1	1:E:296:PHE:HB3	2.43	0.44
1:A:211:GLN:HG3	1:A:249:ILE:HB	1.98	0.44
1:C:192:LEU:N	1:C:192:LEU:CD1	2.80	0.44
1:C:60:GLY:C	1:C:61:MET:HG2	2.38	0.44
1:D:225:PHE:CD2	1:D:225:PHE:C	2.90	0.44
1:D:78:ARG:NH1	1:D:78:ARG:HB2	2.19	0.44
1:A:239:HIS:CE1	1:A:281:ILE:HG21	2.52	0.44
1:B:192:LEU:N	1:B:192:LEU:CD2	2.77	0.44
1:D:125:THR:O	1:D:126:ARG:C	2.56	0.44
1:D:139:TRP:HA	1:D:179:MET:HE2	1.98	0.44
1:E:215:ARG:HG3	1:E:215:ARG:HH11	1.81	0.44
1:E:297:GLN:HG2	1:E:297:GLN:O	2.17	0.44
1:E:303:PRO:O	1:E:304:HIS:ND1	2.50	0.44
1:A:257:ILE:CG2	1:A:265:LEU:CD1	2.95	0.44
1:C:84:VAL:HG22	1:C:225:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLU:OE2	1:D:244:LYS:HD2	2.17	0.44
1:D:216:SER:OG	2:D:314:GSH:N1	2.48	0.44
1:E:161:LEU:O	1:E:165:ILE:HG12	2.17	0.44
1:E:52:GLY:O	1:E:53:THR:HB	2.17	0.44
1:A:57:SER:HB3	1:A:256:HIS:HB3	1.99	0.44
1:B:102:SER:OG	1:B:107:LYS:NZ	2.49	0.44
1:B:283:ARG:CG	1:B:284:LYS:N	2.79	0.44
1:C:107:LYS:HG2	1:C:110:ASP:OD2	2.18	0.44
1:C:31:LEU:CA	1:C:34:LEU:HD12	2.45	0.44
1:D:285:VAL:HG21	1:D:291:PHE:CZ	2.51	0.44
1:E:123:PHE:N	1:E:123:PHE:HD2	2.15	0.44
1:E:90:TRP:NE1	1:E:95:SER:OG	2.51	0.44
1:B:99:LYS:HA	1:B:102:SER:CB	2.48	0.44
1:B:42:ARG:HE	1:B:43:CYS:HG	1.63	0.44
1:C:107:LYS:CG	1:C:110:ASP:OD2	2.66	0.44
1:C:85:LEU:HD12	1:C:232:LEU:HD21	1.99	0.44
1:C:90:TRP:CG	1:C:101:LEU:HD13	2.53	0.44
1:D:162:GLN:OE1	1:D:165:ILE:HD12	2.17	0.44
1:E:294:GLU:H	1:E:294:GLU:CD	2.21	0.44
1:A:32:GLN:O	1:A:36:GLN:HG3	2.18	0.44
1:C:225:PHE:C	1:C:225:PHE:HD2	2.21	0.44
1:C:227:ILE:O	1:C:231:ALA:HB2	2.18	0.44
1:C:235:TYR:CE1	1:C:245:PRO:HG2	2.53	0.44
1:C:55:THR:HG22	1:C:258:TYR:HA	2.00	0.44
1:D:280:ARG:O	1:D:282:LEU:HD22	2.17	0.44
1:D:33:TYR:CE2	1:D:224:PRO:HG3	2.53	0.44
1:D:78:ARG:HH12	1:D:303:PRO:CG	2.21	0.44
1:E:182:TRP:HD1	1:E:182:TRP:O	2.01	0.44
1:D:136:GLY:O	1:D:139:TRP:HB2	2.18	0.43
1:D:56:LEU:HD22	1:D:262:ILE:HD11	2.00	0.43
1:B:187:LEU:HD11	1:B:194:PRO:HD2	2.00	0.43
1:C:232:LEU:O	1:C:235:TYR:HB2	2.18	0.43
1:C:69:ASP:O	1:C:278:LYS:HE3	2.17	0.43
1:D:144:ALA:HB2	1:D:157:GLY:HA3	2.01	0.43
1:E:103:SER:C	1:E:105:GLY:H	2.21	0.43
1:E:142:PHE:CD2	1:E:142:PHE:C	2.91	0.43
1:E:274:ARG:HD2	1:E:304:HIS:CE1	2.54	0.43
1:E:87:GLU:HG2	1:E:91:PHE:CZ	2.53	0.43
1:C:277:PRO:HG3	1:C:301:TYR:HA	2.00	0.43
1:C:75:THR:C	1:C:77:LYS:N	2.71	0.43
1:C:76:THR:OG1	1:C:268:GLN:NE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:SER:OG	1:D:117:PHE:HB2	2.18	0.43
1:D:34:LEU:C	1:D:36:GLN:H	2.22	0.43
1:E:42:ARG:O	1:E:43:CYS:SG	2.73	0.43
1:A:286:GLU:CD	1:D:50:ARG:NH2	2.72	0.43
1:B:53:THR:O	1:B:54:GLY:O	2.36	0.43
1:C:99:LYS:C	1:C:101:LEU:N	2.72	0.43
1:C:161:LEU:O	1:C:164:VAL:HG23	2.18	0.43
1:C:178:ILE:CG2	1:C:179:MET:N	2.81	0.43
1:E:289:ASP:C	1:E:291:PHE:H	2.22	0.43
1:E:289:ASP:O	1:E:291:PHE:N	2.51	0.43
1:E:47:LYS:HG2	1:E:48:ASP:H	1.81	0.43
1:A:74:LEU:HD12	1:A:224:PRO:HB3	1.99	0.43
1:D:178:ILE:HD11	1:D:200:GLN:HG3	1.99	0.43
1:D:88:LEU:HD23	1:D:236:MET:SD	2.57	0.43
1:A:261:HIS:C	1:A:264:PRO:HD2	2.39	0.43
1:B:40:ILE:O	1:B:44:GLY:HA3	2.19	0.43
1:B:87:GLU:HG3	1:B:88:LEU:N	2.32	0.43
1:E:135:TYR:O	1:E:138:GLN:N	2.51	0.43
1:B:96:THR:HG21	1:B:137:PHE:HB2	2.01	0.43
1:C:135:TYR:CZ	1:C:196:HIS:CE1	3.06	0.43
1:C:192:LEU:HD13	1:C:192:LEU:N	2.33	0.43
1:D:187:LEU:C	1:D:189:LEU:H	2.21	0.43
1:D:28:HIS:HD2	1:D:273:PRO:HB2	1.81	0.43
1:D:33:TYR:CZ	1:D:37:ILE:HD11	2.54	0.43
1:E:137:PHE:HZ	1:E:144:ALA:HB3	1.82	0.43
1:E:184:PRO:HA	1:E:187:LEU:HD22	2.00	0.43
1:E:304:HIS:HB3	1:E:305:PRO:CD	2.49	0.43
1:E:49:ASP:OD2	1:E:52:GLY:N	2.51	0.43
1:E:78:ARG:NH1	1:E:78:ARG:CG	2.81	0.43
1:B:161:LEU:CB	1:B:179:MET:HE1	2.48	0.43
1:C:84:VAL:HA	1:C:225:PHE:HE2	1.83	0.43
1:E:214:GLN:OE1	1:E:250:HIS:NE2	2.44	0.43
1:E:223:VAL:HG12	1:E:224:PRO:N	2.34	0.43
1:A:192:LEU:N	1:A:192:LEU:CD1	2.82	0.43
1:B:108:ILE:CD1	1:B:109:TRP:HD1	2.31	0.43
1:B:118:LEU:HB3	1:B:123:PHE:O	2.19	0.43
1:D:162:GLN:O	1:D:164:VAL:N	2.52	0.43
2:D:314:GSH:O12	1:E:176:ARG:NH1	2.52	0.42
1:E:48:ASP:HB3	1:E:49:ASP:H	1.46	0.42
1:A:127:GLU:OE2	1:A:127:GLU:HA	2.19	0.42
1:A:73:LEU:HG	1:A:301:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ILE:HB	1:B:286:GLU:O	2.19	0.42
1:C:102:SER:C	1:C:104:LYS:H	2.22	0.42
1:D:112:ASN:HA	1:D:117:PHE:CD1	2.55	0.42
1:A:287:LYS:HG3	1:D:50:ARG:O	2.20	0.42
1:E:182:TRP:NE1	1:E:184:PRO:HG3	2.34	0.42
1:E:283:ARG:O	1:E:285:VAL:HG23	2.19	0.42
1:E:114:SER:O	1:E:118:LEU:CD1	2.67	0.42
1:E:68:ARG:O	1:E:69:ASP:CB	2.67	0.42
1:B:40:ILE:HG21	1:B:257:ILE:HG13	2.01	0.42
1:C:107:LYS:C	1:C:109:TRP:H	2.23	0.42
1:C:233:LEU:HD12	1:C:233:LEU:O	2.19	0.42
1:C:274:ARG:O	1:C:275:PRO:C	2.57	0.42
1:E:207:GLU:HA	1:E:244:LYS:O	2.19	0.42
1:E:68:ARG:O	1:E:69:ASP:HB2	2.18	0.42
1:B:283:ARG:NE	1:B:285:VAL:HG22	2.34	0.42
1:B:30:GLU:OE2	1:B:75:THR:N	2.34	0.42
1:D:166:ASP:HA	1:D:169:LYS:NZ	2.33	0.42
1:D:92:ILE:C	1:D:94:GLY:H	2.22	0.42
1:E:97:ASN:ND2	1:E:149:MET:SD	2.79	0.42
1:E:37:ILE:HD12	1:E:257:ILE:HD11	2.01	0.42
1:E:77:LYS:HG2	1:E:78:ARG:N	2.35	0.42
1:A:196:HIS:CB	1:A:212:LEU:HD11	2.50	0.42
1:B:102:SER:HA	1:B:106:VAL:O	2.20	0.42
1:D:74:LEU:CD2	1:D:224:PRO:HB3	2.50	0.42
1:E:260:ASN:HB2	1:E:261:HIS:CD2	2.55	0.42
1:E:76:THR:HA	1:E:304:HIS:HD2	1.84	0.42
1:B:147:ARG:NH2	1:B:151:SER:HB2	2.34	0.42
1:D:204:VAL:HG21	1:E:45:VAL:HG21	2.01	0.42
1:B:185:ARG:NH1	1:B:185:ARG:CG	2.77	0.42
1:C:168:ILE:HD13	1:C:208:LEU:CD1	2.48	0.42
1:D:222:GLY:HA3	2:D:314:GSH:HA31	1.98	0.42
1:D:212:LEU:O	1:D:251:THR:HB	2.19	0.42
1:D:262:ILE:HG22	1:D:263:GLU:N	2.35	0.42
1:D:71:PHE:CD1	1:D:71:PHE:C	2.93	0.42
1:E:97:ASN:HD22	1:E:149:MET:HE1	1.83	0.42
1:A:137:PHE:HE1	1:A:153:TYR:CE2	2.37	0.41
1:A:232:LEU:HG	1:A:236:MET:CE	2.50	0.41
1:A:239:HIS:CD2	1:A:239:HIS:C	2.93	0.41
1:B:92:ILE:CD1	1:B:236:MET:HE1	2.50	0.41
1:C:99:LYS:C	1:C:101:LEU:H	2.23	0.41
1:D:177:ILE:C	1:D:178:ILE:HD12	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:LEU:HD11	1:D:194:PRO:HD2	2.02	0.41
1:E:141:HIS:O	1:E:142:PHE:O	2.39	0.41
1:C:196:HIS:CD2	1:C:230:TYR:OH	2.65	0.41
1:D:144:ALA:O	1:D:145:GLU:C	2.58	0.41
1:D:175:ARG:HH11	1:E:215:ARG:HH12	1.68	0.41
1:E:215:ARG:HG3	1:E:215:ARG:NH1	2.35	0.41
1:A:148:ASP:C	1:A:150:GLU:H	2.24	0.41
1:A:259:LEU:HA	1:A:262:ILE:HD11	2.02	0.41
1:C:107:LYS:O	1:C:109:TRP:N	2.54	0.41
1:C:82:LYS:O	1:C:82:LYS:HG2	2.21	0.41
1:D:110:ASP:N	1:D:110:ASP:OD2	2.53	0.41
1:D:141:HIS:HD2	1:D:153:TYR:O	2.03	0.41
1:D:215:ARG:HH12	2:D:314:GSH:HN11	1.68	0.41
1:A:187:LEU:HD23	1:A:190:MET:HE1	2.02	0.41
1:D:286:GLU:HB3	1:D:287:LYS:H	1.56	0.41
1:E:34:LEU:C	1:E:36:GLN:N	2.73	0.41
1:A:171:ASN:O	1:A:174:ASP:HB2	2.21	0.41
1:A:254:ASP:OD2	1:B:202:TYR:HE1	2.03	0.41
1:D:73:LEU:O	1:D:74:LEU:C	2.58	0.41
1:A:183:ASN:HB3	1:A:186:ASP:HB2	2.01	0.41
1:C:102:SER:HA	1:C:106:VAL:O	2.20	0.41
1:E:134:VAL:O	1:E:135:TYR:C	2.59	0.41
1:E:233:LEU:O	1:E:237:ILE:HG13	2.20	0.41
1:A:30:GLU:OE1	1:A:76:THR:HG23	2.20	0.41
1:B:174:ASP:HB3	1:B:177:ILE:HG13	2.03	0.41
1:B:62:GLN:NE2	1:B:211:GLN:NE2	2.69	0.41
1:B:76:THR:O	1:B:268:GLN:HG3	2.20	0.41
1:C:109:TRP:CE3	1:C:131:LEU:HD13	2.56	0.41
1:D:215:ARG:HG3	1:D:215:ARG:NH1	2.35	0.41
1:E:88:LEU:CD2	1:E:232:LEU:HG	2.50	0.41
1:A:202:TYR:HB2	1:B:59:PHE:CD2	2.56	0.41
1:A:271:ARG:HD3	1:A:304:HIS:CG	2.55	0.41
1:B:85:LEU:HD12	1:B:85:LEU:C	2.41	0.41
1:C:219:MET:HB2	1:C:256:HIS:O	2.21	0.41
1:C:249:ILE:CD1	1:C:249:ILE:H	2.33	0.41
1:C:274:ARG:CZ	1:C:304:HIS:CD2	3.04	0.41
1:D:219:MET:SD	1:D:223:VAL:HG21	2.61	0.41
1:A:213:TYR:CD1	1:A:213:TYR:C	2.94	0.41
1:B:118:LEU:H	1:B:118:LEU:CD1	2.32	0.41
1:B:182:TRP:CE3	1:B:194:PRO:HG2	2.56	0.41
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:VAL:HG12	1:C:108:ILE:HG12	2.01	0.41
1:C:161:LEU:HA	1:C:164:VAL:HG23	2.02	0.41
1:D:87:GLU:O	1:D:90:TRP:HB3	2.21	0.41
1:E:115:ARG:NH1	1:E:124:SER:HA	2.36	0.41
1:A:68:ARG:NH1	1:A:247:ASP:OD2	2.54	0.41
1:C:167:THR:O	1:C:168:ILE:C	2.58	0.41
1:C:249:ILE:HD12	1:C:249:ILE:H	1.85	0.41
1:C:71:PHE:O	1:C:73:LEU:N	2.51	0.41
1:A:46:ARG:HA	1:A:55:THR:O	2.21	0.41
1:B:88:LEU:HA	1:B:91:PHE:HD2	1.85	0.41
1:C:160:GLN:O	1:C:164:VAL:HG22	2.21	0.41
1:C:193:PRO:HA	1:C:194:PRO:HD3	1.94	0.41
1:C:218:ASP:C	1:C:218:ASP:OD2	2.60	0.41
1:D:191:ALA:O	1:D:192:LEU:HB2	2.21	0.41
1:E:288:ILE:O	1:E:291:PHE:HD2	2.04	0.41
1:A:147:ARG:HB2	1:A:151:SER:OG	2.21	0.40
1:B:174:ASP:OD2	1:B:176:ARG:HG2	2.21	0.40
1:B:48:ASP:HB3	1:B:52:GLY:HA2	2.01	0.40
1:D:178:ILE:HD12	1:D:200:GLN:HG3	2.02	0.40
1:D:208:LEU:CD2	1:D:237:ILE:HG22	2.52	0.40
1:E:223:VAL:CB	1:E:224:PRO:HD3	2.51	0.40
1:B:115:ARG:HD3	1:B:115:ARG:C	2.41	0.40
1:B:133:PRO:HG3	1:B:146:TYR:CG	2.56	0.40
1:B:164:VAL:HG11	1:B:201:PHE:CD2	2.56	0.40
1:D:240:ILE:HG23	1:D:240:ILE:O	2.22	0.40
1:D:283:ARG:HG2	1:D:295:ASP:OD2	2.21	0.40
1:D:277:PRO:HB3	1:D:301:TYR:N	2.36	0.40
1:D:178:ILE:HG21	1:E:182:TRP:CE2	2.57	0.40
1:E:177:ILE:CG2	1:E:201:PHE:HB2	2.52	0.40
1:A:73:LEU:HD11	1:A:79:VAL:HB	2.02	0.40
1:C:198:LEU:HD13	1:C:199:CYS:N	2.37	0.40
1:D:240:ILE:HD11	1:D:287:LYS:O	2.22	0.40
1:D:184:PRO:HD2	1:E:142:PHE:CZ	2.56	0.40
1:E:219:MET:HB2	1:E:257:ILE:HG12	2.04	0.40
1:E:88:LEU:HD23	1:E:232:LEU:CD2	2.52	0.40
1:E:74:LEU:HD12	1:E:224:PRO:CB	2.45	0.40

There are no symmetry-related clashes.

## 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	279/313 (89%)	243 (87%)	30 (11%)	6 (2%)	6	11
1	B	279/313 (89%)	236 (85%)	31 (11%)	12 (4%)	2	3
1	C	278/313 (89%)	231 (83%)	33 (12%)	14 (5%)	2	2
1	D	279/313 (89%)	207 (74%)	52 (19%)	20 (7%)	1	1
1	E	278/313 (89%)	200 (72%)	49 (18%)	29 (10%)	0	0
All	All	1393/1565 (89%)	1117 (80%)	195 (14%)	81 (6%)	1	1

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	54	GLY
1	B	114	SER
1	B	135	TYR
1	C	103	SER
1	D	126	ARG
1	D	240	ILE
1	D	305	PRO
1	E	45	VAL
1	E	53	THR
1	E	108	ILE
1	E	128	GLU
1	E	135	TYR
1	E	142	PHE
1	A	80	PHE
1	B	80	PHE
1	B	261	HIS
1	C	74	LEU
1	D	157	GLY
1	D	286	GLU
1	D	294	GLU
1	E	54	GLY

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Mol	Chain	Res	Type
1	E	154	SER
1	E	260	ASN
1	E	290	ASP
1	A	72	PRO
1	B	44	GLY
1	B	197	ALA
1	C	52	GLY
1	C	76	THR
1	C	108	ILE
1	C	205	ASN
1	C	220	GLY
1	C	239	HIS
1	C	275	PRO
1	C	277	PRO
1	D	125	THR
1	D	145	GLU
1	D	222	GLY
1	D	303	PRO
1	E	38	GLN
1	E	43	CYS
1	E	69	ASP
1	E	107	LYS
1	E	227	ILE
1	E	303	PRO
1	A	277	PRO
1	B	77	LYS
1	B	115	ARG
1	B	277	PRO
1	C	72	PRO
1	D	74	LEU
1	D	163	LYS
1	D	188	PRO
1	D	219	MET
1	E	42	ARG
1	E	48	ASP
1	E	49	ASP
1	E	115	ARG
1	E	149	MET
1	E	275	PRO
1	A	115	ARG
1	A	155	GLY
1	A	282	LEU

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Mol	Chain	Res	Type
1	C	133	PRO
1	D	27	PRO
1	D	134	VAL
1	D	236	MET
1	E	28	HIS
1	E	51	THR
1	E	58	VAL
1	E	133	PRO
1	E	269	LEU
1	B	223	VAL
1	C	240	ILE
1	E	130	ASP
1	E	277	PRO
1	B	133	PRO
1	D	277	PRO
1	C	27	PRO
1	D	192	LEU
1	D	143	GLY

### 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	245/271 (90%)	230 (94%)	15 (6%)	18	33
1	B	245/271 (90%)	223 (91%)	22 (9%)	9	16
1	C	244/271 (90%)	222 (91%)	22 (9%)	9	16
1	D	245/271 (90%)	212 (86%)	33 (14%)	4	5
1	E	244/271 (90%)	221 (91%)	23 (9%)	8	15
All	All	1223/1355 (90%)	1108 (91%)	115 (9%)	8	15

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG

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Mol	Chain	Res	Type
1	A	103	SER
1	A	104	LYS
1	A	127	GLU
1	A	152	ASP
1	A	189	LEU
1	A	192	LEU
1	A	195	CYS
1	A	196	HIS
1	A	198	LEU
1	A	204	VAL
1	A	221	LEU
1	A	250	HIS
1	A	297	GLN
1	A	302	ASN
1	B	46	ARG
1	B	69	ASP
1	B	78	ARG
1	B	86	GLU
1	B	87	GLU
1	B	89	LEU
1	B	100	GLU
1	B	108	ILE
1	B	110	ASP
1	B	126	ARG
1	B	128	GLU
1	B	176	ARG
1	B	226	ASN
1	B	240	ILE
1	B	247	ASP
1	B	259	LEU
1	B	260	ASN
1	B	266	LYS
1	B	269	LEU
1	B	281	ILE
1	B	284	LYS
1	B	299	GLU
1	C	32	GLN
1	C	34	LEU
1	C	48	ASP
1	C	61	MET
1	C	115	ARG
1	C	117	PHE

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Mol	Chain	Res	Type
1	C	119	ASP
1	C	125	THR
1	C	164	VAL
1	C	176	ARG
1	C	187	LEU
1	C	192	LEU
1	C	198	LEU
1	C	210	CYS
1	C	221	LEU
1	C	225	PHE
1	C	229	SER
1	C	274	ARG
1	C	275	PRO
1	C	283	ARG
1	C	290	ASP
1	C	302	ASN
1	D	38	GLN
1	D	41	LEU
1	D	50	ARG
1	D	56	LEU
1	D	68	ARG
1	D	69	ASP
1	D	78	ARG
1	D	85	LEU
1	D	100	GLU
1	D	115	ARG
1	D	125	THR
1	D	140	ARG
1	D	145	GLU
1	D	149	MET
1	D	160	GLN
1	D	174	ASP
1	D	178	ILE
1	D	179	MET
1	D	187	LEU
1	D	196	HIS
1	D	209	SER
1	D	225	PHE
1	D	240	ILE
1	D	249	ILE
1	D	270	GLN
1	D	281	ILE

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Mol	Chain	Res	Type
1	D	283	ARG
1	D	286	GLU
1	D	287	LYS
1	D	289	ASP
1	D	292	LYS
1	D	294	GLU
1	D	296	PHE
1	E	50	ARG
1	E	69	ASP
1	E	78	ARG
1	E	96	THR
1	E	100	GLU
1	E	104	LYS
1	E	107	LYS
1	E	116	ASP
1	E	118	LEU
1	E	119	ASP
1	E	134	VAL
1	E	135	TYR
1	E	174	ASP
1	E	198	LEU
1	E	252	LEU
1	E	256	HIS
1	E	260	ASN
1	E	261	HIS
1	E	263	GLU
1	E	275	PRO
1	E	283	ARG
1	E	296	PHE
1	E	299	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	112	ASN
1	A	171	ASN
1	A	196	HIS
1	A	205	ASN
1	A	302	ASN
1	B	32	GLN
1	B	39	HIS

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Mol	Chain	Res	Type
1	B	97	ASN
1	B	112	ASN
1	B	156	GLN
1	B	160	GLN
1	B	171	ASN
1	B	196	HIS
1	B	205	ASN
1	B	211	GLN
1	B	256	HIS
1	C	28	HIS
1	C	32	GLN
1	C	38	GLN
1	C	112	ASN
1	C	138	GLN
1	C	196	HIS
1	C	200	GLN
1	C	205	ASN
1	C	211	GLN
1	C	268	GLN
1	C	297	GLN
1	C	302	ASN
1	D	28	HIS
1	D	32	GLN
1	D	36	GLN
1	D	38	GLN
1	D	97	ASN
1	D	112	ASN
1	D	141	HIS
1	D	156	GLN
1	D	160	GLN
1	D	200	GLN
1	D	211	GLN
1	E	38	GLN
1	E	62	GLN
1	E	156	GLN
1	E	196	HIS
1	E	200	GLN
1	E	226	ASN
1	E	261	HIS
1	E	304	HIS



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 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$
3	PO4	C	365	-	4,4,4	1.70	1 (25%)	6,6,6	0.42	0
2	GSH	A	581	-	12,19,19	0.97	0	15,24,24	2.01	5 (33%)
2	GSH	D	314	1	12,19,19	1.50	2 (16%)	15,24,24	5.82	13 (86%)
3	PO4	A	365	-	4,4,4	1.61	0	6,6,6	0.47	0
3	PO4	E	366	-	4,4,4	1.64	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSH	A	581	-	-	2/18/24/24	-
2	GSH	D	314	1	-	4/18/24/24	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	314	GSH	CA2-C2	-2.98	1.45	1.52
2	D	314	GSH	CD1-N2	-2.11	1.29	1.34
3	C	365	PO4	P-O2	-2.06	1.48	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	314	GSH	CA3-N3-C2	11.46	138.82	122.34
2	D	314	GSH	CG1-CD1-N2	-8.41	101.25	115.83
2	D	314	GSH	CA2-N2-CD1	7.79	141.69	121.65
2	D	314	GSH	C2-CA2-N2	7.27	130.94	111.16
2	D	314	GSH	CG1-CB1-CA1	-6.82	97.94	113.84
2	D	314	GSH	OE1-CD1-N2	5.08	131.52	122.95
2	D	314	GSH	CB2-CA2-N2	-5.02	104.13	111.28
2	D	314	GSH	CB1-CG1-CD1	4.77	123.70	113.04
2	D	314	GSH	CA2-CB2-SG2	-4.54	109.09	114.19
2	D	314	GSH	CA2-C2-N3	-4.49	107.49	116.54
2	A	581	GSH	CA2-C2-N3	4.17	124.96	116.54
2	D	314	GSH	C3-CA3-N3	-3.42	103.83	110.43
2	A	581	GSH	C2-CA2-N2	-3.34	102.07	111.16
2	D	314	GSH	OE1-CD1-CG1	2.82	127.17	122.02
2	A	581	GSH	O2-C2-N3	-2.81	116.95	122.99
2	D	314	GSH	O2-C2-CA2	2.60	125.93	120.45
2	A	581	GSH	CB2-CA2-N2	-2.36	107.91	111.28
2	A	581	GSH	CG1-CB1-CA1	-2.36	108.34	113.84

There are no chirality outliers.

All (6) torsion outliers are listed below:

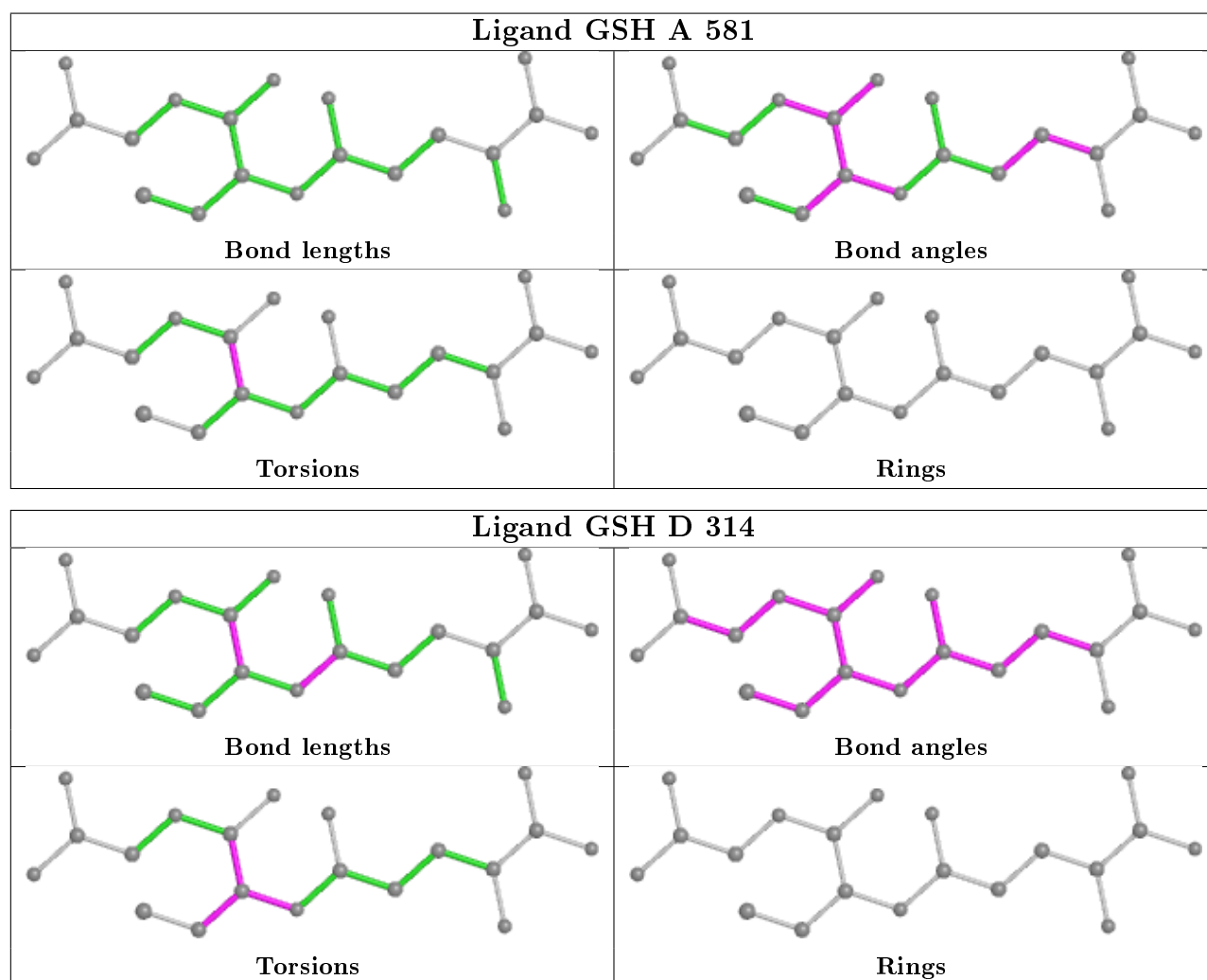
Mol	Chain	Res	Type	Atoms
2	D	314	GSH	C2-CA2-N2-CD1
2	D	314	GSH	N2-CA2-CB2-SG2
2	A	581	GSH	O2-C2-CA2-N2
2	A	581	GSH	N3-C2-CA2-N2
2	D	314	GSH	O2-C2-CA2-N2
2	D	314	GSH	N3-C2-CA2-N2

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	314	GSH	10	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.



## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	281/313 (89%)	-0.04	1 (0%) 92 95	40, 65, 98, 114	0
1	B	281/313 (89%)	0.17	13 (4%) 32 39	42, 83, 126, 142	0
1	C	280/313 (89%)	0.21	8 (2%) 51 61	42, 83, 128, 153	0
1	D	281/313 (89%)	0.50	24 (8%) 10 13	49, 110, 137, 159	0
1	E	280/313 (89%)	0.42	16 (5%) 23 28	54, 110, 154, 165	0
All	All	1403/1565 (89%)	0.25	62 (4%) 34 41	40, 88, 136, 165	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	144	ALA	4.6
1	C	74	LEU	4.3
1	D	89	LEU	4.0
1	B	123	PHE	3.8
1	B	306	THR	3.8
1	D	298	ILE	3.7
1	B	114	SER	3.7
1	D	291	PHE	3.5
1	D	282	LEU	3.4
1	D	290	ASP	3.4
1	B	147	ARG	3.4
1	D	281	ILE	3.2
1	D	137	PHE	3.2
1	C	258	TYR	3.2
1	B	126	ARG	3.2
1	D	299	GLU	3.1
1	D	276	PHE	3.1
1	D	204	VAL	3.1
1	D	277	PRO	3.1
1	E	270	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	221	LEU	3.0
1	B	127	GLU	2.9
1	B	116	ASP	2.9
1	E	257	ILE	2.9
1	E	267	ILE	2.9
1	D	300	GLY	2.8
1	D	279	LEU	2.7
1	B	128	GLU	2.6
1	D	288	ILE	2.6
1	B	73	LEU	2.6
1	E	41	LEU	2.6
1	D	106	VAL	2.5
1	E	34	LEU	2.4
1	E	300	GLY	2.4
1	C	267	ILE	2.4
1	C	251	THR	2.4
1	E	153	TYR	2.3
1	B	74	LEU	2.3
1	B	221	LEU	2.3
1	E	74	LEU	2.3
1	B	265	LEU	2.2
1	C	271	ARG	2.2
1	D	85	LEU	2.2
1	B	272	GLU	2.2
1	C	60	GLY	2.2
1	D	296	PHE	2.2
1	A	31	LEU	2.2
1	E	277	PRO	2.2
1	D	202	TYR	2.1
1	D	297	GLN	2.1
1	C	56	LEU	2.1
1	D	72	PRO	2.1
1	D	120	SER	2.1
1	D	65	TYR	2.1
1	D	230	TYR	2.1
1	E	268	GLN	2.1
1	E	266	LYS	2.1
1	E	191	ALA	2.0
1	E	269	LEU	2.0
1	E	263	GLU	2.0
1	C	252	LEU	2.0
1	D	272	GLU	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](#)

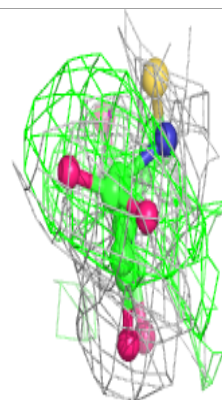
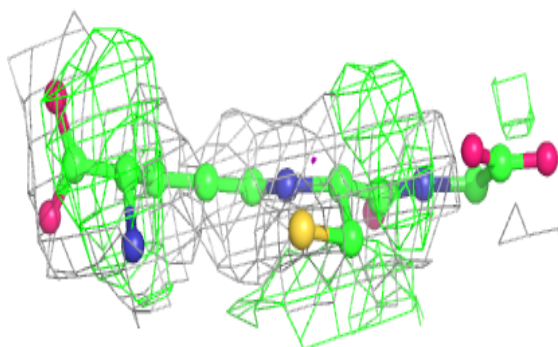
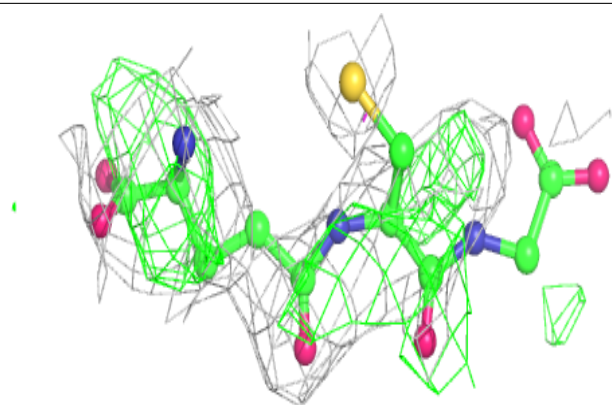
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	GSH	D	314	20/20	0.69	0.55	63,102,125,128	20
3	PO4	E	366	5/5	0.86	0.22	148,150,151,152	0
2	GSH	A	581	20/20	0.87	0.36	46,118,153,154	0
3	PO4	C	365	5/5	0.91	0.19	118,119,120,122	0
3	PO4	A	365	5/5	0.96	0.18	87,89,90,94	0

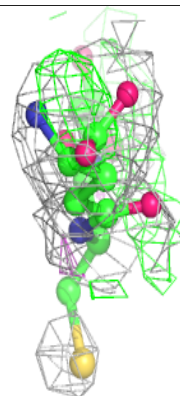
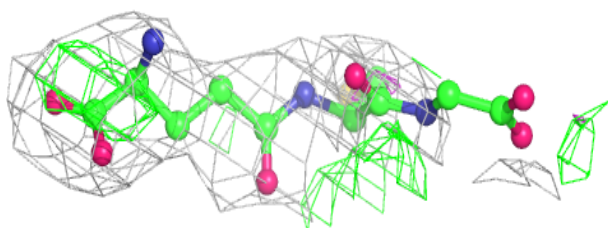
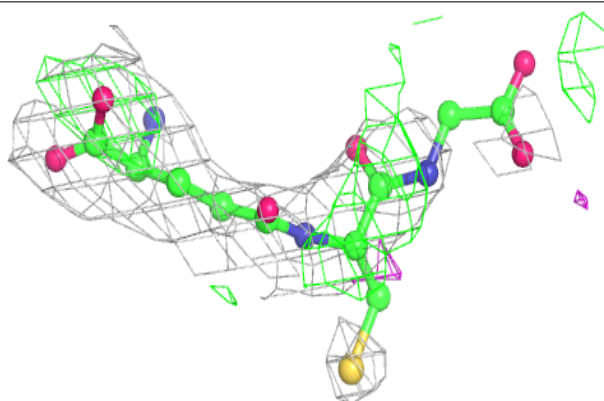
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around GSH D 314:**

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

**Electron density around GSH A 581:**

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





## 6.5 Other polymers

There are no such residues in this entry.