



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:41 PM UTC

PDB ID : 3OB7 / pdb_00003ob7
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

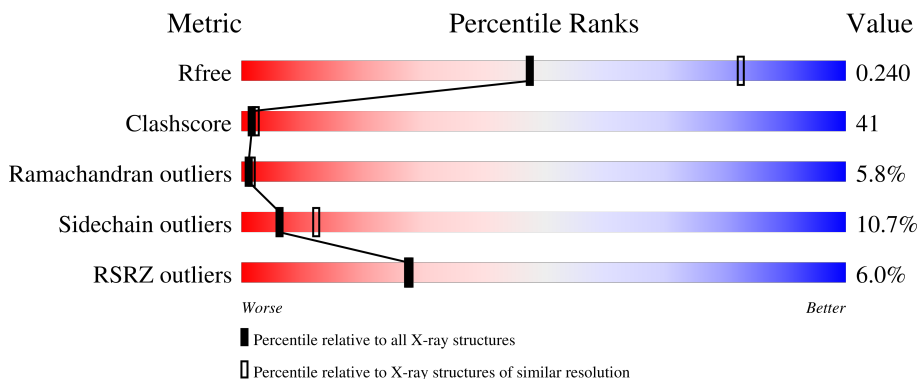
1 Overall quality at a glance

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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	313	
1	C	313	
1	D	313	
1	E	313	

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	-

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.

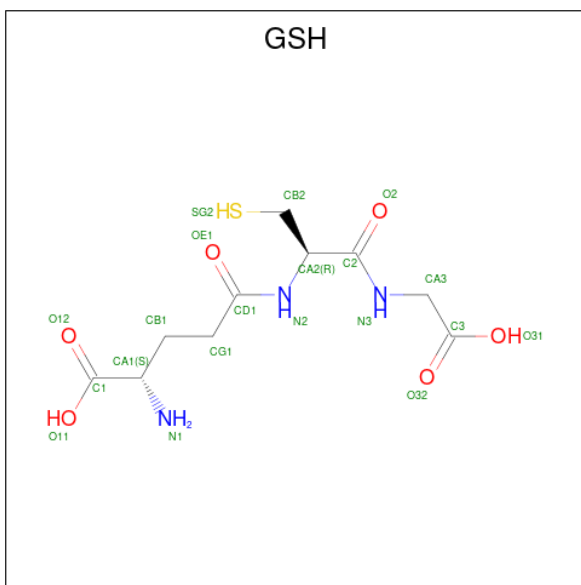
- Molecule 1 is a protein called Thymidylate synthase.

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:

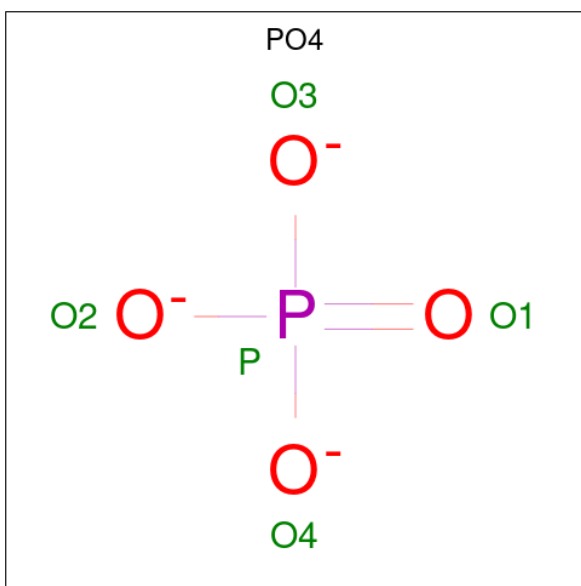
Chain	Residue	Modelled	Actual	Comment	Reference
A	163	LYS	ARG	engineered mutation	UNP P04818
B	163	LYS	ARG	engineered mutation	UNP P04818
C	163	LYS	ARG	engineered mutation	UNP P04818
D	163	LYS	ARG	engineered mutation	UNP P04818
E	163	LYS	ARG	engineered mutation	UNP P04818

- Molecule 2 is GLUTATHIONE (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



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 (CCD ID: PO4) (formula: O_4P).



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

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

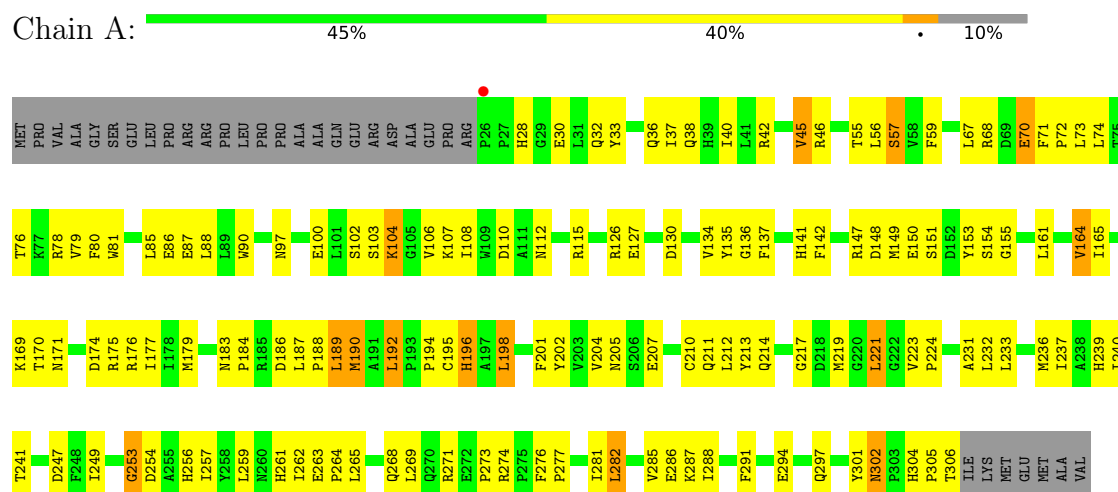
- Molecule 4 is water.

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		

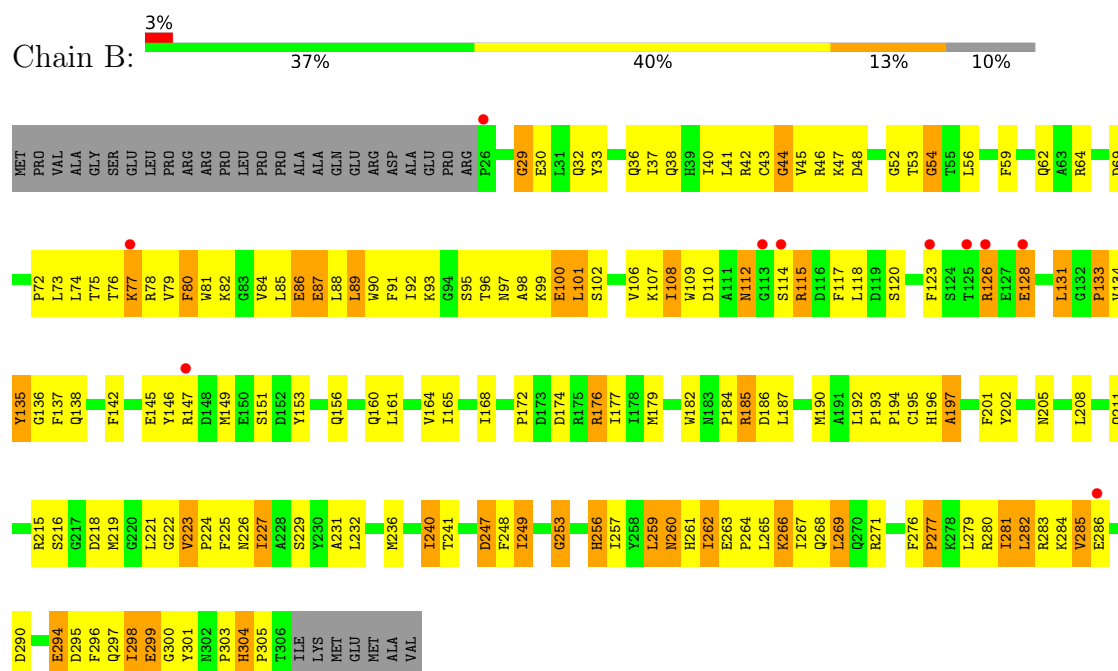
3 Residue-property plots

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

• Molecule 1: Thymidylate synthase

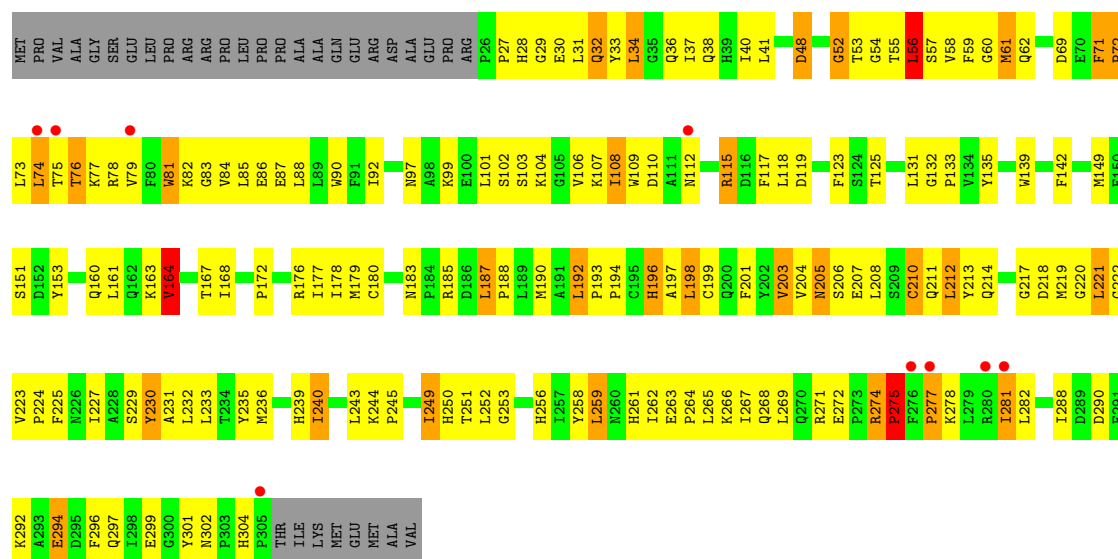


• Molecule 1: Thymidylate synthase



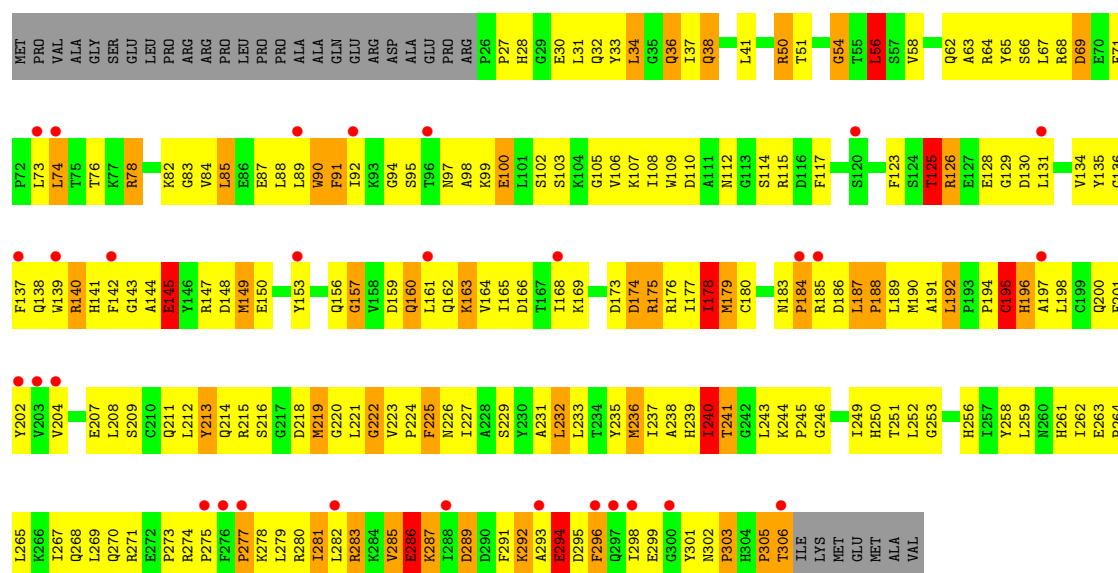
• Molecule 1: Thymidylate synthase

Chain C: 3% 37% 42% 9% 11%



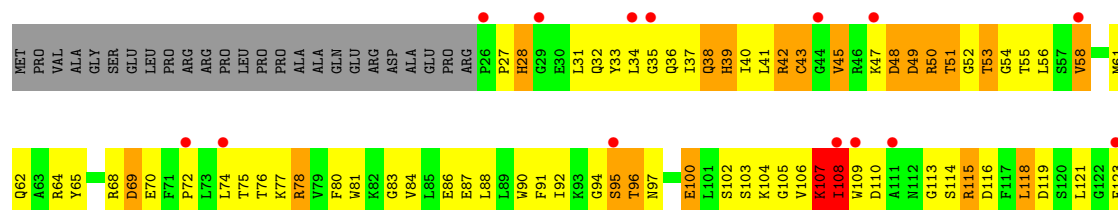
• Molecule 1: Thymidylate synthase

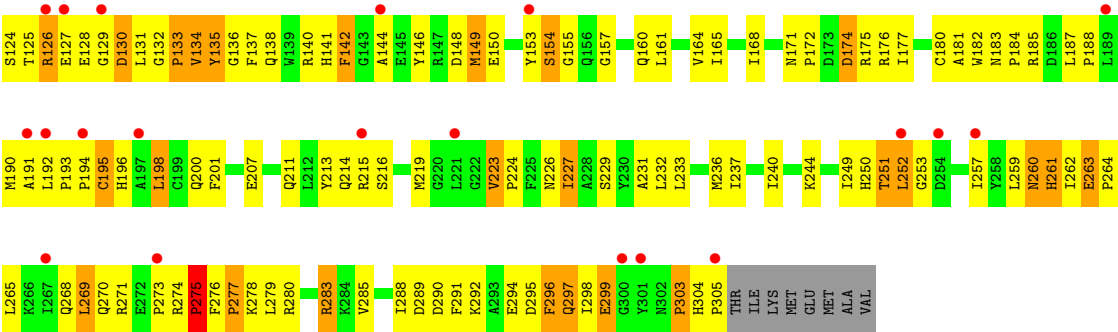
Chain D: 10% 26% 47% 14% 10%



• Molecule 1: Thymidylate synthase

Chain E: 11% 29% 45% 14% 11%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.80Å 123.11Å 99.93Å 90.00° 115.75° 90.00°	Depositor
Resolution (Å)	45.46 – 2.75 45.46 – 2.75	Depositor EDS
% Data completeness (in resolution range)	78.7 (45.46-2.75) 82.7 (45.46-2.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.293 0.245 , 0.240	Depositor DCC
R_{free} test set	5126 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 68.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.56	0/2328	1.04	9/3150 (0.3%)
1	B	0.46	0/2328	1.01	11/3150 (0.3%)
1	C	0.49	0/2321	1.05	13/3140 (0.4%)
1	D	0.44	0/2328	1.09	18/3150 (0.6%)
1	E	0.43	0/2321	1.01	10/3140 (0.3%)
All	All	0.48	0/11626	1.04	61/15730 (0.4%)

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 (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	196	HIS	N-CA-C	-10.84	88.32	107.28
1	D	34	LEU	N-CA-C	-10.48	95.88	110.35
1	D	103	SER	N-CA-C	-10.14	101.03	113.50
1	D	195	CYS	CA-C-O	-10.04	110.53	121.78
1	E	231	ALA	N-CA-C	-8.80	101.59	111.71
1	D	241	THR	N-CA-C	-8.27	102.08	114.64
1	D	178	ILE	N-CA-C	8.13	119.41	108.27
1	C	56	LEU	N-CA-C	-7.93	97.72	110.32
1	B	253	GLY	N-CA-C	-7.59	103.30	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	SER	N-CA-C	7.43	120.37	109.07
1	D	285	VAL	N-CA-C	7.40	119.26	108.53
1	C	266	LYS	N-CA-C	-7.12	103.53	111.28
1	A	253	GLY	N-CA-C	-7.06	103.78	110.21
1	C	132	GLY	CA-C-N	6.99	128.57	119.84
1	C	132	GLY	C-N-CA	6.99	128.57	119.84
1	A	231	ALA	N-CA-C	-6.94	103.65	111.14
1	D	256	HIS	N-CA-C	6.80	119.51	109.24
1	E	195	CYS	N-CA-C	-6.67	105.11	113.18
1	E	95	SER	N-CA-C	6.60	118.89	108.67
1	E	108	ILE	N-CA-C	6.54	122.94	109.34
1	B	231	ALA	N-CA-C	-6.53	104.09	111.07
1	D	91	PHE	N-CA-C	-6.47	104.15	111.14
1	D	36	GLN	N-CA-C	-6.46	103.52	111.40
1	E	94	GLY	N-CA-C	-6.29	105.67	115.67
1	B	262	ILE	N-CA-C	6.25	117.00	110.62
1	B	300	GLY	N-CA-C	-6.20	106.39	115.63
1	A	56	LEU	N-CA-C	-6.20	99.09	109.07
1	E	39	HIS	N-CA-C	-6.19	104.80	112.72
1	B	29	GLY	N-CA-C	6.01	119.91	112.64
1	B	256	HIS	N-CA-C	6.01	118.54	109.41
1	D	195	CYS	O-C-N	-5.96	113.88	121.92
1	E	126	ARG	N-CA-C	5.94	119.16	109.24
1	A	108	ILE	N-CA-C	5.91	120.71	112.50
1	D	31	LEU	N-CA-C	-5.88	105.95	113.01
1	A	71	PHE	CA-C-N	5.83	127.13	119.84
1	A	71	PHE	C-N-CA	5.83	127.13	119.84
1	C	164	VAL	N-CA-C	-5.80	104.85	110.42
1	D	108	ILE	N-CA-C	5.80	116.45	110.36
1	C	71	PHE	CA-C-N	5.66	126.92	119.84
1	C	71	PHE	C-N-CA	5.66	126.92	119.84
1	D	232	LEU	N-CA-C	-5.60	105.17	112.23
1	C	57	SER	N-CA-C	5.57	118.28	108.75
1	B	101	LEU	N-CA-C	-5.57	106.49	113.28
1	B	227	ILE	N-CA-C	-5.53	104.94	110.30
1	E	155	GLY	N-CA-C	-5.47	107.72	115.43
1	B	195	CYS	N-CA-C	-5.47	106.45	113.23
1	D	90	TRP	N-CA-C	-5.41	106.81	113.41
1	A	85	LEU	N-CA-C	5.39	116.97	111.14
1	D	56	LEU	N-CA-C	-5.38	100.53	109.46
1	B	285	VAL	N-CA-C	5.37	117.36	108.99
1	C	183	ASN	CA-C-N	5.28	125.33	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ASN	C-N-CA	5.28	125.33	119.32
1	C	81	TRP	N-CA-C	5.16	117.58	111.33
1	D	231	ALA	N-CA-C	-5.16	99.81	110.80
1	E	297	GLN	N-CA-C	5.14	115.82	107.23
1	D	54	GLY	N-CA-C	5.12	120.69	111.62
1	C	33	TYR	N-CA-C	5.11	117.24	111.11
1	E	180	CYS	N-CA-C	5.06	116.76	108.52
1	A	67	LEU	N-CA-C	-5.05	106.53	113.30
1	B	131	LEU	N-CA-C	5.04	119.13	112.89
1	C	203	VAL	N-CA-C	5.01	115.66	107.24

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 [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	2268	0	2235	110	0
1	B	2268	0	2235	183	0
1	C	2261	0	2228	166	0
1	D	2268	0	2234	257	0
1	E	2261	0	2228	248	0
2	A	20	0	15	0	0
2	D	20	0	12	11	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	16	0	0	1	0
All	All	11445	0	11187	930	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 41.

All (930) 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:HD13	1:D:281:ILE:H	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
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:HD23	1:B:192:LEU:H	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:HG3	1:B:185:ARG:HH11	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:123:PHE:HZ	1:D:189:LEU:HA	1.44	0.83
1:D:160:GLN:O	1:D:164:VAL:HG23	1.79	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:H	1:E:135:TYR:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:187:LEU:HA	1:A:190:MET:HE2	1.65	0.78
1:C:109:TRP:CZ3	1:C:192:LEU:HD11	2.19	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:185:ARG:O	1:E:188:PRO:HD2	1.83	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
1:B:161:LEU:HA	1:B:179:MET:HE2	1.66	0.76
1:D:214:GLN:HB3	1:D:252:LEU:HD23	1.67	0.76
1:E:77:LYS:HD3	1:E:78:ARG:H	1.47	0.76
1:E:268:GLN:HG3	1:E:271:ARG:HD2	1.67	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:B:161:LEU:HD13	1:B:179:MET:HE1	1.68	0.74
1:E:182:TRP:O	1:E:184:PRO:HD3	1.86	0.74
1:B:281:ILE:HD12	1:B:281:ILE:N	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:OD2	1:D:289:ASP:N	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:31:LEU:HA	1:C:34:LEU:HD12	1.71	0.73
1:C:164:VAL:HG12	1:C:177:ILE:HG22	1.71	0.73
1:C:222:GLY:H	1:C:224:PRO:HD2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:74:LEU:HD22	1:D:74:LEU:H	1.54	0.71
1:D:198:LEU:HD11	1:E:213:TYR:CD1	2.26	0.71
1:B:92:ILE:CD1	1:B:236:MET:HE1	2.21	0.70
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
1:E:77:LYS:CD	1:E:78:ARG:H	2.05	0.70
1:C:41:LEU:HD23	1:C:56:LEU:HD22	1.74	0.70
1:C:249:ILE:HD12	1:C:249:ILE:N	2.07	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:E:190:MET:HE1	1:E:194:PRO:HG3	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:E:127:GLU:H	1:E:127:GLU:CD	1.99	0.69
1:B:279:LEU:HD11	1:B:296:PHE:HB3	1.73	0.69
1:E:148:ASP:C	1:E:150:GLU:H	2.00	0.69
1:E:132:GLY:HA2	1:E:146:TYR:CE2	2.27	0.69
1:A:190:MET:HE1	1:A:194:PRO:HD3	1.73	0.69
1:B:285:VAL:HG11	1:B:290:ASP:HB2	1.75	0.69
1:D:281:ILE:HD13	1:D:281:ILE:N	2.02	0.69
1:E:118:LEU:H	1:E:118:LEU:CD1	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:H	1:D:74:LEU:CD2	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:37:ILE:C	1:E:39:HIS:H	2.01	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:49:ASP:CG	1:E:53:THR:HG22	2.19	0.67
1:E:47:LYS:CG	1:E:48:ASP:H	2.08	0.66
1:E:183:ASN:O	1:E:187:LEU:HB2	1.95	0.66
1:A:86:GLU:HG2	1:A:104:LYS:HB2	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
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:C:294:GLU:H	1:C:294:GLU:CD	2.02	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:96:THR:HG22	1:E:132:GLY:O	1.97	0.65
1:E:135:TYR:HE1	1:E:196:HIS:HD2	1.45	0.65
1:D:195:CYS:O	1:D:195:CYS:SG	2.55	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:127:GLU:CD	1:E:127:GLU:N	2.54	0.64
1:B:161:LEU:HA	1:B:179:MET:CE	2.27	0.64
1:D:32:GLN:NE2	1:D:64:ARG:H	1.92	0.64
1:D:305:PRO:O	1:D:306:THR:HG23	1.98	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: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:HB2	1:D:169:LYS:NZ	2.14	0.63
1:D:187:LEU:HA	1:D:190:MET:HE3	1.80	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
1:B:82:LYS:O	1:B:86:GLU:HB2	1.98	0.62
1:B:153:TYR:HA	1:B:156:GLN:NE2	2.15	0.62
1:B:87:GLU:HA	1:B:101:LEU:HD21	1.82	0.62
1:B:161:LEU:CA	1:B:179:MET:HE2	2.29	0.62
1:A:88:LEU:HD23	1:A:236:MET:HE3	1.82	0.61
1:D:50:ARG:HB3	1:D:50:ARG:NH2	2.13	0.61
1:D:282:LEU:H	1:D:282:LEU:HD22	1.65	0.61
1:D:89:LEU:O	1:D:89:LEU:HD23	2.00	0.61
1:E:97:ASN:HD22	1:E:149:MET:HE1	1.65	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:D:198:LEU:HD12	1:D:198:LEU:C	2.25	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:235:TYR:C	1:D:237:ILE:H	2.06	0.61
1:D:50:ARG:HD2	2:D:314:GSH:O12	2.00	0.61
1:E:97:ASN:ND2	1:E:149:MET:HE1	2.16	0.61
1:D:200:GLN:HE22	1:E:253:GLY:HA3	1.66	0.61
1:D:33:TYR:HB2	1:D:65:TYR:OH	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:HIS:HD2	4:D:319:HOH:O	1.84	0.61
1:E:118:LEU:HD23	1:E:126:ARG:CB	2.31	0.60
1:B:281:ILE:H	1:B:281:ILE:CD1	2.13	0.60
1:C:41:LEU:HA	1:C:56:LEU:CD2	2.32	0.60
1:D:140:ARG:HG3	1:D:140:ARG:HH11	1.66	0.60
1:D:253:GLY:HA3	1:E:200:GLN:HE22	1.66	0.60
1:E:35:GLY:HA2	1:E:38:GLN:HG2	1.83	0.60
1:E:92:ILE:CD1	1:E:236:MET:HE1	2.31	0.60
1:E:132:GLY:O	1:E:134:VAL:HG22	2.01	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:E:268:GLN:C	1:E:270:GLN:H	2.08	0.60
1:C:232:LEU:HG	1:C:236:MET:HE3	1.83	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:30:GLU:OE1	1:B:76:THR:HG23	2.02	0.59
1:B:72:PRO:HA	1:B:276:PHE:CD1	2.37	0.59
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: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:HD23	1:B:192:LEU:N	2.13	0.59
1:D:221:LEU:HD11	1:D:261:HIS:HE1	1.66	0.59
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:E:198:LEU:C	1:E:198:LEU:HD12	2.26	0.59
1:D:173:ASP:N	1:D:173:ASP:OD1	2.35	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:A:198:LEU:C	1:A:198:LEU:HD12	2.27	0.59
1:E:133:PRO:HG3	1:E:146:TYR:CG	2.38	0.59
1:C:53:THR:HG22	1:C:54:GLY:N	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:PRO:O	1:C:267:ILE:HB	2.03	0.59
1:D:83:GLY:HA2	1:D:106:VAL:CG2	2.32	0.59
1:D:280:ARG:O	1:D:296:PHE:HA	2.03	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:HG3	1:B:185:ARG:NH1	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:B:161:LEU:CD1	1:B:179:MET:HE1	2.32	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:B:187:LEU:HA	1:B:190:MET:HE3	1.86	0.58
1:D:30:GLU:OE1	1:D:74:LEU:HA	2.04	0.58
1:D:279:LEU:HD11	1:D:296:PHE:HB3	1.86	0.58
1:E:31:LEU:HD23	1:E:273:PRO:HG2	1.86	0.58
1:E:149:MET:HE3	1:E:149:MET:O	2.04	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
1:C:139:TRP:CE2	1:C:179:MET:HE3	2.39	0.58
1:D:294:GLU:CD	1:D:294:GLU:H	2.12	0.58
1:E:127:GLU:C	1:E:129:GLY:H	2.11	0.57
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:E:87:GLU:O	1:E:90:TRP:HB3	2.04	0.57
1:E:261:HIS:N	1:E:261:HIS:CD2	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:HD23	1:A:236:MET:CE	2.34	0.57
1:C:222:GLY:C	1:C:224:PRO:HD2	2.29	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:HD13	1:B:101:LEU:O	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:C:84:VAL:HG22	1:C:225:PHE:CD2	2.40	0.56
1:D:294:GLU:CD	1:D:294:GLU:N	2.63	0.56
1:E:118:LEU:HD12	1:E:118:LEU:N	2.08	0.56
1:B:117:PHE:O	1:B:120:SER:HB3	2.05	0.56
1:D:74:LEU:HD22	1:D:74:LEU:N	2.20	0.56
1:D:176:ARG:HD3	1:E:193:PRO:CG	2.33	0.56
1:A:38:GLN:CG	1:A:269:LEU:HD13	2.36	0.56
1:E:97:ASN:HB2	1:E:149:MET:SD	2.45	0.56
1:E:252:LEU:HD12	1:E:252:LEU:H	1.70	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:97:ASN:ND2	1:C:149:MET:SD	2.79	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:B:264:PRO:O	1:B:267:ILE:HG12	2.05	0.56
1:E:35:GLY:HA2	1:E:38:GLN:NE2	2.20	0.56
1:E:75:THR:O	1:E:303:PRO:HA	2.06	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:B:84:VAL:HG13	1:B:229:SER:HA	1.88	0.55
1:B:40:ILE:HD12	1:B:219:MET:HG3	1.88	0.55
1:A:305:PRO:O	1:A:306:THR:HB	2.05	0.55
1:C:75:THR:C	1:C:77:LYS:H	2.12	0.55
1:D:66:SER:C	1:D:67:LEU:HD12	2.30	0.55
1:E:80:PHE:HE2	1:E:106:VAL:HG13	1.70	0.55
1:E:213:TYR:CD2	1:E:251:THR:HG22	2.40	0.55
1:C:192:LEU:HD22	1:C:192:LEU:O	2.07	0.55
1:D:240:ILE:HD11	1:D:287:LYS:C	2.32	0.55
1:E:76:THR:O	1:E:271:ARG:HD3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:141:HIS:O	1:E:142:PHE:C	2.50	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:E:263:GLU:H	1:E:263:GLU:CD	2.12	0.55
1:B:135:TYR:O	1:B:136:GLY:C	2.50	0.55
1:E:41:LEU:HA	1:E:56:LEU:HD23	1.88	0.55
1:E:240:ILE:HD11	1:E:291:PHE:HE2	1.72	0.55
1:E:261:HIS:C	1:E:264:PRO:HD2	2.31	0.55
1:D:34:LEU:HD22	1:D:269:LEU:HD12	1.89	0.54
1:D:240:ILE:HD12	1:D:291:PHE:HE2	1.72	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:HB2	1:D:169:LYS:HZ2	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:N	1:A:221:LEU:HD22	2.23	0.54
1:B:115:ARG:O	1:B:115:ARG:HD3	2.08	0.54
1:E:252:LEU:HD12	1:E:252:LEU:N	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: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:D:135:TYR:O	1:D:139:TRP:CD1	2.60	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:286:GLU:OE2	1:D:50:ARG:NH2	2.42	0.53
1:B:88:LEU:HA	1:B:91:PHE:CD2	2.43	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:C:264:PRO:HA	1:C:267:ILE:HD12	1.90	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:175:ARG:O	1:E:215:ARG:HD2	2.07	0.53
1:E:92:ILE:HD11	1:E:236:MET:HE1	1.91	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:50:ARG:O	1:E:51:THR:HG23	2.08	0.53
1:E:130:ASP:HB2	1:E:149:MET:HG2	1.89	0.53
1:E:153:TYR:O	1:E:154:SER:C	2.51	0.53
1:D:281:ILE:HG12	1:D:281:ILE:O	2.09	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:D:139:TRP:CG	1:D:179:MET:HE1	2.44	0.53
1:D:190:MET:C	1:D:192:LEU:H	2.16	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: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
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:A:68:ARG:C	1:A:70:GLU:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HD11	1:B:109:TRP:HD1	1.74	0.52
1:A:45:VAL:HG21	1:B:205:ASN:HD21	1.74	0.52
1:E:47:LYS:CG	1:E:48:ASP:N	2.73	0.52
1:E:304:HIS:HB3	1:E:305:PRO:HD2	1.91	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:235:TYR:C	1:D:237:ILE:N	2.68	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:HD12	1:B:118:LEU:H	1.75	0.52
1:E:38:GLN:HB3	1:E:269:LEU:HD21	1.91	0.52
1:E:196:HIS:HE1	1:E:226:ASN:CG	2.18	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:HH11	1:D:78:ARG:CB	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:102:SER:HB3	1:D:110:ASP:CG	2.34	0.51
1:D:261:HIS:O	1:D:264:PRO:HG2	2.09	0.51
1:E:78:ARG:HG3	1:E:78:ARG:NH1	2.21	0.51
1:E:240:ILE:CD1	1:E:288:ILE:HA	2.38	0.51
1:B:44:GLY:O	1:B:56:LEU:HD22	2.10	0.51
1:B:112:ASN:H	1:B:112:ASN:HD22	1.57	0.51
1:B:135:TYR:O	1:B:138:GLN:N	2.42	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:HH11	1:B:185:ARG:CG	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLN:HG3	1:E:61:MET:HE1	1.93	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:40:ILE:HA	1:E:58:VAL:HG21	1.93	0.50
1:E:119:ASP:HA	1:E:124:SER:OG	2.11	0.50
1:B:294:GLU:CD	1:B:294:GLU:H	2.17	0.50
1:E:74:LEU:CD1	1:E:224:PRO:HB3	2.39	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:190:MET:HE1	1:E:194:PRO:CG	2.39	0.50
1:A:79:VAL:O	1:A:81:TRP:N	2.44	0.50
1:B:53:THR:O	1:B:53:THR:HG22	2.11	0.50
1:B:97:ASN:ND2	1:B:100:GLU:H	2.10	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: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:C:225:PHE:CD2	1:C:225:PHE:C	2.90	0.49
1:A:70:GLU:HG2	1:A:276:PHE:HB2	1.93	0.49
1:B:196:HIS:O	1:B:197:ALA:C	2.55	0.49
1:B:248:PHE:C	1:B:249:ILE:HD13	2.37	0.49
1:D:140:ARG:HG3	1:D:140:ARG:NH1	2.27	0.49
1:C:87:GLU:O	1:C:90:TRP:HB3	2.13	0.49
1:C:187:LEU:HD12	1:C:188:PRO:HD3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185:ARG:C	1:E:187:LEU:H	2.19	0.49
1:D:141:HIS:O	1:D:142:PHE:C	2.55	0.49
1:D:187:LEU:HB2	1:D:188:PRO:HD3	1.95	0.49
1:E:41:LEU:HD23	1:E:56:LEU:HD22	1.94	0.49
1:E:55:THR:C	1:E:56:LEU:HD12	2.37	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:E:294:GLU:CD	1:E:294:GLU:H	2.21	0.49
1:A:88:LEU:CD2	1:A:236:MET:HE3	2.41	0.49
1:C:29:GLY:O	1:C:32:GLN:HB2	2.13	0.49
1:C:60:GLY:C	1:C:61:MET:HG2	2.38	0.49
1:D:125:THR:O	1:D:126:ARG:C	2.56	0.49
1:D:225:PHE:C	1:D:225:PHE:CD2	2.90	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:CG	1:B:160:GLN:NE2	2.76	0.49
1:A:184:PRO:HD2	1:B:142:PHE:CZ	2.48	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:A:170:THR:HG22	1:D:258:TYR:CD1	2.48	0.48
1:B:259:LEU:HD12	1:B:262:ILE:HD11	1.95	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:103:SER:C	1:E:105:GLY:H	2.21	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: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:B:263:GLU:OE2	1:B:266:LYS:HE3	2.13	0.48
1:C:117:PHE:HD2	1:C:117:PHE:O	1.97	0.48
1:C:206:SER:O	1:C:243:LEU:HB3	2.13	0.48
1:D:187:LEU:N	1:D:190:MET:HE3	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:GLU:CD	1:D:50:ARG:NH2	2.72	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
1:C:225:PHE:HD2	1:C:225:PHE:C	2.21	0.48
1:E:108:ILE:HG23	1:E:109:TRP:N	2.27	0.48
1:E:142:PHE:C	1:E:142:PHE:CD2	2.91	0.48
1:A:33:TYR:CE1	1:A:74:LEU:HD13	2.48	0.48
1:E:148:ASP:C	1:E:150:GLU:N	2.67	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:C:75:THR:C	1:C:77:LYS:N	2.71	0.48
1:D:109:TRP:CE3	1:D:131:LEU:HD13	2.48	0.48
1:A:261:HIS:C	1:A:264:PRO:HD2	2.39	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:D:34:LEU:C	1:D:36:GLN:H	2.22	0.48
1:D:187:LEU:C	1:D:189:LEU:H	2.21	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:73:LEU:HG	1:A:301:TYR:CE1	2.49	0.47
1:A:192:LEU:N	1:A:192:LEU:HD13	2.29	0.47
1:C:263:GLU:O	1:C:267:ILE:HG13	2.14	0.47
1:D:287:LYS:HB2	1:D:287:LYS:HZ3	1.78	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:E:289:ASP:C	1:E:291:PHE:H	2.22	0.47
1:C:99:LYS:C	1:C:101:LEU:N	2.72	0.47
1:C:102:SER:C	1:C:104:LYS:H	2.22	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:177:ILE:C	1:D:178:ILE:HD12	2.40	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:164:VAL:HG12	1:A:165:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:HIS:O	1:A:264:PRO:HD2	2.15	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:B:118:LEU:HD12	1:B:118:LEU:N	2.28	0.47
1:C:74:LEU:CD1	1:C:224:PRO:HB3	2.39	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:HD12	1:D:67:LEU:N	2.30	0.47
1:D:92:ILE:C	1:D:94:GLY:N	2.70	0.47
1:E:116:ASP:O	1:E:119:ASP:HB2	2.14	0.47
1:E:135:TYR:CD2	1:E:135:TYR:N	2.74	0.47
1:E:187:LEU:N	1:E:188:PRO:HD2	2.28	0.47
1:A:259:LEU:O	1:A:262:ILE:HG13	2.15	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:92:ILE:C	1:D:94:GLY:H	2.22	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:58:VAL:CG1	1:C:59:PHE:N	2.78	0.47
1:C:219:MET:HA	1:C:223:VAL:HG21	1.95	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:C:107:LYS:C	1:C:109:TRP:H	2.23	0.46
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:71:PHE:CD1	1:D:71:PHE:C	2.93	0.46
1:D:187:LEU:CA	1:D:190:MET:HE3	2.45	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:A:239:HIS:C	1:A:239:HIS:CD2	2.93	0.46
1:C:75:THR:O	1:C:77:LYS:N	2.48	0.46
1:C:274:ARG:O	1:C:275:PRO:C	2.57	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:D:144:ALA:O	1:D:145:GLU:C	2.58	0.46
1:E:107:LYS:H	1:E:107:LYS:CE	2.27	0.46
1:A:148:ASP:C	1:A:150:GLU:H	2.24	0.46
1:A:151:SER:HB2	1:A:153:TYR:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:TRP:O	1:D:95:SER:HB3	2.16	0.46
1:D:198:LEU:HD12	1:D:198:LEU:O	2.14	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:E:31:LEU:CD2	1:E:273:PRO:HG2	2.45	0.46
1:E:34:LEU:C	1:E:36:GLN:N	2.73	0.46
1:B:240:ILE:O	1:B:240:ILE:HG13	2.16	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:40:ILE:O	1:E:56:LEU:HD23	2.15	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: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:134:VAL:O	1:E:135:TYR:C	2.59	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:115:ARG:HD3	1:B:115:ARG:C	2.41	0.46
1:B:123:PHE:HB3	1:B:126:ARG:HG3	1.97	0.46
1:B:216:SER:OG	1:B:256:HIS:HE1	1.99	0.46
1:D:296:PHE:CD1	1:D:296:PHE:N	2.83	0.46
1:E:62:GLN:HA	1:E:250:HIS:O	2.16	0.46
1:E:125:THR:HG22	1:E:125:THR:O	2.16	0.46
1:A:107:LYS:HA	1:A:110:ASP:OD2	2.16	0.46
1:B:85:LEU:HD12	1:B:85:LEU:C	2.41	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:88:LEU:HD21	1:D:233:LEU:HD13	1.97	0.46
1:D:148:ASP:N	1:D:153:TYR:OH	2.49	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:97:ASN:HB2	1:A:149:MET:SD	2.56	0.45
1:A:213:TYR:CD1	1:A:213:TYR:C	2.94	0.45
1:A:214:GLN:HE21	1:A:217:GLY:HA3	1.81	0.45
1:B:88:LEU:HD13	1:B:232:LEU:HD23	1.97	0.45
1:B:215:ARG:HG3	1:B:216:SER:H	1.81	0.45
1:C:167:THR:O	1:C:168:ILE:C	2.58	0.45
1:C:78:ARG:HA	1:C:301:TYR:OH	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:O	1:C:188:PRO:HD2	2.15	0.45
1:C:218:ASP:OD2	1:C:218:ASP:C	2.60	0.45
1:D:97:ASN:HD22	1:D:100:GLU:H	1.64	0.45
1:D:123:PHE:CD2	1:D:123:PHE:N	2.83	0.45
1:B:36:GLN:O	1:B:40:ILE:HG13	2.16	0.45
1:B:128:GLU:OE1	1:B:128:GLU:O	2.34	0.45
1:D:163:LYS:O	1:D:163:LYS:HD3	2.17	0.45
1:E:38:GLN:CB	1:E:269:LEU:HD21	2.46	0.45
1:E:211:GLN:HB2	1:E:249:ILE:HB	1.97	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:E:268:GLN:C	1:E:270:GLN:N	2.75	0.45
1:C:48:ASP:OD2	1:C:52:GLY:HA2	2.16	0.45
1:C:88:LEU:HD23	1:C:236:MET:HE3	1.97	0.45
1:C:99:LYS:C	1:C:101:LEU:H	2.23	0.45
1:C:292:LYS:HB3	1:C:294:GLU:OE2	2.17	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:47:LYS:HG3	1:E:48:ASP:H	1.77	0.45
1:E:261:HIS:O	1:E:265:LEU:HG	2.15	0.45
1:D:73:LEU:O	1:D:74:LEU:C	2.58	0.45
1:D:198:LEU:HD11	1:E:213:TYR:CE1	2.51	0.45
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:30:GLU:C	1:D:32:GLN:N	2.75	0.45
1:D:139:TRP:HA	1:D:179:MET:CE	2.47	0.45
1:C:62:GLN:O	1:C:62:GLN:HG2	2.16	0.45
1:D:62:GLN:NE2	1:D:211:GLN:NE2	2.64	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:E:72:PRO:HA	1:E:276:PHE:CE1	2.52	0.45
1:E:211:GLN:HA	1:E:249:ILE:O	2.16	0.45
1:B:263:GLU:HB2	1:B:264:PRO:HD3	1.98	0.45
1:D:32:GLN:HG3	1:D:63:ALA:HB1	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:B:62:GLN:NE2	1:B:211:GLN:HE22	2.15	0.45
1:D:219:MET:HE1	1:D:252:LEU:HD13	1.99	0.45
1:E:49:ASP:HB3	1:E:52:GLY:N	2.32	0.45
1:E:276:PHE:HD1	1:E:277:PRO:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:PHE:HA	1:A:253:GLY:O	2.17	0.44
1:A:78:ARG:HH11	1:A:78:ARG:HG3	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:37:ILE:C	1:E:39:HIS:N	2.68	0.44
1:A:68:ARG:HE	1:A:207:GLU:CD	2.26	0.44
1:A:161:LEU:HA	1:A:179:MET:HE2	1.99	0.44
1:A:134:VAL:O	1:A:135:TYR:C	2.59	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:B:142:PHE:C	1:B:142:PHE:CD2	2.95	0.44
1:C:192:LEU:CD1	1:C:192:LEU:N	2.80	0.44
1:D:78:ARG:HB2	1:D:78:ARG:NH1	2.19	0.44
1:D:293:ALA:C	1:D:295:ASP:H	2.25	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:E:215:ARG:HG3	1:E:215:ARG:HH11	1.81	0.44
1:E:297:GLN:O	1:E:297:GLN:HG2	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:B:187:LEU:N	1:B:190:MET:HE3	2.33	0.44
1:C:84:VAL:HG22	1:C:225:PHE:CE2	2.53	0.44
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:52:GLY:O	1:E:53:THR:HB	2.17	0.44
1:E:161:LEU:O	1:E:165:ILE:HG12	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:31:LEU:CA	1:C:34:LEU:HD12	2.45	0.44
1:C:107:LYS:HG2	1:C:110:ASP:OD2	2.18	0.44
1:D:285:VAL:HG21	1:D:291:PHE:CZ	2.51	0.44
1:D:287:LYS:HB2	1:D:287:LYS:HZ2	1.82	0.44
1:E:90:TRP:NE1	1:E:95:SER:OG	2.51	0.44
1:E:123:PHE:N	1:E:123:PHE:HD2	2.15	0.44
1:B:42:ARG:HE	1:B:43:CYS:HG	1.63	0.44
1:B:99:LYS:HA	1:B:102:SER:CB	2.48	0.44
1:B:134:VAL:O	1:B:135:TYR:C	2.61	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:C:107:LYS:CG	1:C:110:ASP:OD2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:GLN:OE1	1:D:165:ILE:HD12	2.17	0.44
1:D:198:LEU:C	1:D:198:LEU:CD1	2.90	0.44
1:A:30:GLU:CD	1:A:76:THR:HG23	2.43	0.44
1:A:32:GLN:O	1:A:36:GLN:HG3	2.18	0.44
1:A:294:GLU:CD	1:A:294:GLU:H	2.24	0.44
1:C:55:THR:HG22	1:C:258:TYR:HA	2.00	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: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:D:280:ARG:O	1:D:282:LEU:HD22	2.17	0.44
1:E:182:TRP:O	1:E:182:TRP:HD1	2.01	0.44
1:D:56:LEU:HD22	1:D:262:ILE:HD11	2.00	0.43
1:D:136:GLY:O	1:D:139:TRP:HB2	2.18	0.43
1:B:187:LEU:HD11	1:B:194:PRO:HD2	2.00	0.43
1:C:69:ASP:O	1:C:278:LYS:HE3	2.17	0.43
1:C:232:LEU:O	1:C:235:TYR:HB2	2.18	0.43
1:D:139:TRP:HA	1:D:179:MET:HE1	2.00	0.43
1:D:144:ALA:HB2	1:D:157:GLY:HA3	2.01	0.43
1:E:27:PRO:O	1:E:28:HIS:C	2.61	0.43
1:E:87:GLU:HG2	1:E:91:PHE:CZ	2.53	0.43
1:E:274:ARG:HD2	1:E:304:HIS:CE1	2.54	0.43
1:C:76:THR:OG1	1:C:268:GLN:NE2	2.48	0.43
1:C:277:PRO:HG3	1:C:301:TYR:HA	2.00	0.43
1:D:114:SER:OG	1:D:117:PHE:HB2	2.18	0.43
1:E:42:ARG:O	1:E:43:CYS:SG	2.73	0.43
1:B:53:THR:O	1:B:54:GLY:O	2.36	0.43
1:B:222:GLY:O	1:B:223:VAL:C	2.60	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:D:54:GLY:C	1:D:259:LEU:HG	2.43	0.43
1:E:47:LYS:HG2	1:E:48:ASP:H	1.81	0.43
1:E:289:ASP:O	1:E:291:PHE:N	2.51	0.43
1:A:74:LEU:HD12	1:A:224:PRO:HB3	1.99	0.43
1:D:88:LEU:HD23	1:D:236:MET:SD	2.57	0.43
1:D:178:ILE:HD11	1:D:200:GLN:HG3	1.99	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:D:226:ASN:O	1:D:227:ILE:C	2.61	0.43
1:E:135:TYR:O	1:E:138:GLN:N	2.51	0.43
1:B:92:ILE:HD11	1:B:236:MET:HE1	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:28:HIS:HD2	1:D:273:PRO:HB2	1.81	0.43
1:D:30:GLU:C	1:D:32:GLN:H	2.25	0.43
1:D:33:TYR:CZ	1:D:37:ILE:HD11	2.54	0.43
1:D:222:GLY:C	2:D:314:GSH:HA32	2.44	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: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:C:84:VAL:HA	1:C:225:PHE:HE2	1.83	0.43
1:D:98:ALA:O	1:D:99:LYS:C	2.62	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:D:265:LEU:C	1:D:267:ILE:N	2.75	0.43
1:B:92:ILE:HD13	1:B:236:MET:HE1	1.97	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:C:81:TRP:C	1:C:83:GLY:N	2.77	0.43
1:D:162:GLN:O	1:D:164:VAL:N	2.52	0.43
1:B:75:THR:C	1:B:77:LYS:H	2.28	0.42
1:C:294:GLU:CD	1:C:294:GLU:N	2.74	0.42
1:D:139:TRP:CB	1:D:179:MET:HE1	2.48	0.42
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:73:LEU:HG	1:A:301:TYR:CZ	2.55	0.42
1:A:287:LYS:HG3	1:D:50:ARG:O	2.20	0.42
1:B:240:ILE:HB	1:B:286:GLU:O	2.19	0.42
1:D:112:ASN:HA	1:D:117:PHE:CD1	2.55	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:B:260:ASN:C	1:B:262:ILE:H	2.27	0.42
1:E:114:SER:O	1:E:118:LEU:CD1	2.67	0.42
1:B:187:LEU:CA	1:B:190:MET:HE3	2.49	0.42
1:E:68:ARG:O	1:E:69:ASP:CB	2.67	0.42
1:E:121:LEU:C	1:E:123:PHE:H	2.27	0.42
1:B:40:ILE:HG21	1:B:257:ILE:HG13	2.01	0.42
1:C:192:LEU:HD22	1:C:192:LEU:C	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:O	1:C:205:ASN:C	2.63	0.42
1:C:233:LEU:HD12	1:C:233:LEU:O	2.19	0.42
1:E:68:ARG:O	1:E:69:ASP:HB2	2.18	0.42
1:E:171:ASN:O	1:E:172:PRO:C	2.63	0.42
1:E:207:GLU:HA	1:E:244:LYS:O	2.19	0.42
1:B:30:GLU:OE2	1:B:75:THR:N	2.34	0.42
1:B:33:TYR:CD1	1:B:33:TYR:C	2.98	0.42
1:B:283:ARG:NE	1:B:285:VAL:HG22	2.34	0.42
1:D:83:GLY:O	1:D:84:VAL:C	2.61	0.42
1:D:166:ASP:HA	1:D:169:LYS:NZ	2.33	0.42
1:A:153:TYR:O	1:A:154:SER:C	2.62	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:E:97:ASN:ND2	1:E:149:MET:SD	2.79	0.42
1:E:185:ARG:C	1:E:187:LEU:N	2.78	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:76:THR:HA	1:E:304:HIS:HD2	1.84	0.42
1:E:260:ASN:HB2	1:E:261:HIS:CD2	2.55	0.42
1:A:240:ILE:HD12	1:A:286:GLU:C	2.44	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:A:127:GLU:OE2	1:A:127:GLU:HA	2.19	0.42
1:A:232:LEU:HG	1:A:236:MET:CE	2.50	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:212:LEU:O	1:D:251:THR:HB	2.19	0.42
1:D:222:GLY:HA3	2:D:314:GSH:HA31	1.98	0.42
1:D:262:ILE:HG22	1:D:263:GLU:N	2.35	0.42
1:D:301:TYR:C	1:D:303:PRO:HD3	2.44	0.42
1:A:137:PHE:HE1	1:A:153:TYR:CE2	2.37	0.41
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: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:126:ARG:HD3	1:A:130:ASP:CG	2.45	0.41
1:A:259:LEU:HA	1:A:262:ILE:HD11	2.02	0.41
1:C:82:LYS:HG2	1:C:82:LYS:O	2.21	0.41
1:C:107:LYS:O	1:C:109:TRP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASP:OD2	1:D:110:ASP:N	2.53	0.41
1:D:141:HIS:HD2	1:D:153:TYR:O	2.03	0.41
1:D:162:GLN:C	1:D:164:VAL:N	2.76	0.41
1:D:215:ARG:HH12	2:D:314:GSH:HN11	1.68	0.41
1:D:239:HIS:CD2	1:D:239:HIS:C	2.98	0.41
1:E:135:TYR:O	1:E:136:GLY:C	2.63	0.41
1:D:277:PRO:O	1:D:278:LYS:C	2.63	0.41
1:D:286:GLU:HB3	1:D:287:LYS:H	1.56	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:A:183:ASN:O	1:A:184:PRO:C	2.64	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: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: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:B:174:ASP:HB3	1:B:177:ILE:HG13	2.03	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:186:ASP:C	1:B:190:MET:HE3	2.45	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:218:ASP:CG	1:D:221:LEU:HB2	2.45	0.41
1:D:219:MET:SD	1:D:223:VAL:HG21	2.61	0.41
1:A:68:ARG:NH1	1:A:247:ASP:OD2	2.54	0.41
1:A:135:TYR:O	1:A:136:GLY:C	2.62	0.41
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.92	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:C:71:PHE:O	1:C:73:LEU:N	2.51	0.41
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:C:249:ILE:HD12	1:C:249:ILE:H	1.85	0.41
1:D:34:LEU:C	1:D:36:GLN:N	2.79	0.41
1:D:87:GLU:O	1:D:90:TRP:HB3	2.21	0.41
1:D:190:MET:C	1:D:192:LEU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:ARG:NH1	1:E:124:SER:HA	2.36	0.41
1:E:274:ARG:O	1:E:275:PRO:C	2.63	0.41
1:A:46:ARG:HA	1:A:55:THR:O	2.21	0.41
1:A:141:HIS:O	1:A:142:PHE:C	2.62	0.41
1:A:232:LEU:HG	1:A:236:MET:HE3	2.03	0.41
1:B:88:LEU:HA	1:B:91:PHE:HD2	1.85	0.41
1:C:117:PHE:C	1:C:117:PHE:CD2	2.98	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:D:191:ALA:O	1:D:192:LEU:HB2	2.21	0.41
1:E:160:GLN:O	1:E:161:LEU:C	2.64	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:48:ASP:HB3	1:B:52:GLY:HA2	2.01	0.40
1:B:174:ASP:OD2	1:B:176:ARG:HG2	2.21	0.40
1:D:178:ILE:HD12	1:D:200:GLN:HG3	2.02	0.40
1:E:289:ASP:C	1:E:291:PHE:N	2.79	0.40
1:A:190:MET:CE	1:A:194:PRO:HD3	2.45	0.40
1:C:142:PHE:CD2	1:C:142:PHE:C	2.99	0.40
1:D:208:LEU:CD2	1:D:237:ILE:HG22	2.52	0.40
1:E:81:TRP:C	1:E:83:GLY:N	2.77	0.40
1:E:223:VAL:CB	1:E:224:PRO:HD3	2.51	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:C:54:GLY:C	1:C:259:LEU:HD13	2.46	0.40
1:D:178:ILE:HG21	1:E:182:TRP:CE2	2.57	0.40
1:D:240:ILE:O	1:D:240:ILE:HG23	2.22	0.40
1:D:277:PRO:HB3	1:D:301:TYR:N	2.36	0.40
1:D:283:ARG:HG2	1:D:295:ASP:OD2	2.21	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:184:PRO:HD2	1:E:142:PHE:CZ	2.56	0.40
1:D:240:ILE:HD11	1:D:287:LYS:O	2.22	0.40
1:E:74:LEU:HD12	1:E:224:PRO:CB	2.45	0.40
1:E:88:LEU:HD23	1:E:232:LEU:CD2	2.52	0.40
1:E:219:MET:HB2	1:E:257:ILE:HG12	2.04	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%)	5	10
1	B	279/313 (89%)	236 (85%)	31 (11%)	12 (4%)	2	3
1	C	278/313 (89%)	231 (83%)	33 (12%)	14 (5%)	1	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	2

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%)	227 (93%)	18 (7%)	13	24
1	B	245/271 (90%)	215 (88%)	30 (12%)	5	8
1	C	244/271 (90%)	218 (89%)	26 (11%)	6	12
1	D	245/271 (90%)	208 (85%)	37 (15%)	3	4
1	E	244/271 (90%)	224 (92%)	20 (8%)	10	20
All	All	1223/1355 (90%)	1092 (89%)	131 (11%)	6	12

All (131) 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	45	VAL
1	A	70	GLU
1	A	100	GLU
1	A	103	SER
1	A	104	LYS
1	A	164	VAL
1	A	175	ARG
1	A	189	LEU
1	A	190	MET
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	297	GLN
1	A	302	ASN
1	B	41	LEU
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	112	ASN
1	B	126	ARG
1	B	128	GLU
1	B	145	GLU
1	B	149	MET
1	B	176	ARG
1	B	185	ARG
1	B	226	ASN
1	B	240	ILE
1	B	247	ASP
1	B	249	ILE
1	B	259	LEU
1	B	260	ASN
1	B	266	LYS
1	B	269	LEU
1	B	281	ILE

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Mol	Chain	Res	Type
1	B	282	LEU
1	B	294	GLU
1	B	298	ILE
1	B	299	GLU
1	B	304	HIS
1	C	32	GLN
1	C	34	LEU
1	C	48	ASP
1	C	56	LEU
1	C	61	MET
1	C	115	ARG
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	196	HIS
1	C	198	LEU
1	C	210	CYS
1	C	212	LEU
1	C	221	LEU
1	C	229	SER
1	C	249	ILE
1	C	259	LEU
1	C	274	ARG
1	C	275	PRO
1	C	281	ILE
1	C	290	ASP
1	C	294	GLU
1	C	302	ASN
1	D	38	GLN
1	D	41	LEU
1	D	50	ARG
1	D	56	LEU
1	D	58	VAL
1	D	69	ASP
1	D	78	ARG
1	D	85	LEU
1	D	100	GLU
1	D	115	ARG
1	D	125	THR

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Mol	Chain	Res	Type
1	D	140	ARG
1	D	145	GLU
1	D	149	MET
1	D	160	GLN
1	D	174	ASP
1	D	175	ARG
1	D	178	ILE
1	D	179	MET
1	D	184	PRO
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
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	D	298	ILE
1	D	306	THR
1	E	50	ARG
1	E	78	ARG
1	E	96	THR
1	E	100	GLU
1	E	104	LYS
1	E	107	LYS
1	E	118	LEU
1	E	134	VAL
1	E	174	ASP
1	E	198	LEU
1	E	223	VAL
1	E	251	THR
1	E	252	LEU
1	E	261	HIS
1	E	263	GLU
1	E	275	PRO

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Mol	Chain	Res	Type
1	E	280	ARG
1	E	283	ARG
1	E	296	PHE
1	E	299	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	38	GLN
1	A	62	GLN
1	A	97	ASN
1	A	112	ASN
1	A	171	ASN
1	A	196	HIS
1	A	205	ASN
1	A	214	GLN
1	A	226	ASN
1	A	302	ASN
1	B	32	GLN
1	B	39	HIS
1	B	62	GLN
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	138	GLN
1	C	141	HIS
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

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Mol	Chain	Res	Type
1	D	32	GLN
1	D	36	GLN
1	D	38	GLN
1	D	62	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	D	302	ASN
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	302	ASN
1	E	304	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	1.76	2 (50%)	6,6,6	0.45	0
3	PO4	E	366	-	4,4,4	1.69	0	6,6,6	0.48	0
2	GSH	A	581	-	18,19,19	1.50	2 (11%)	21,24,24	1.72	5 (23%)
3	PO4	A	365	-	4,4,4	1.66	0	6,6,6	0.50	0
2	GSH	D	314	1	18,19,19	1.66	4 (22%)	21,24,24	4.50	13 (61%)

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	D	314	1	-	5/24/24/24	-
2	GSH	A	581	-	-	7/24/24/24	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	581	GSH	O11-C1	-3.74	1.18	1.30
2	D	314	GSH	O12-C1	3.48	1.32	1.22
2	A	581	GSH	O12-C1	3.37	1.32	1.22
2	D	314	GSH	CA2-C2	-3.10	1.45	1.52
2	D	314	GSH	O11-C1	-3.05	1.20	1.30
3	C	365	PO4	P-O2	-2.14	1.48	1.54
2	D	314	GSH	CD1-N2	-2.12	1.29	1.34
3	C	365	PO4	P-O3	-2.02	1.48	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	314	GSH	CG1-CD1-N2	-8.29	101.25	115.86
2	D	314	GSH	CA2-N2-CD1	7.98	141.69	121.68
2	D	314	GSH	C2-CA2-N2	7.33	130.94	111.11
2	D	314	GSH	CG1-CB1-CA1	-6.94	97.94	113.86
2	D	314	GSH	CA3-N3-C2	6.91	138.82	121.38
2	D	314	GSH	OE1-CD1-N2	5.06	131.52	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	314	GSH	CB2-CA2-N2	-5.02	104.13	111.28
2	D	314	GSH	CB1-CG1-CD1	4.77	123.70	113.06
2	D	314	GSH	CA2-CB2-SG2	-4.50	109.09	114.16
2	D	314	GSH	CA2-C2-N3	-4.21	107.49	116.54
2	A	581	GSH	CA2-C2-N3	3.92	124.96	116.54
2	A	581	GSH	C2-CA2-N2	-3.34	102.07	111.11
2	D	314	GSH	C3-CA3-N3	-2.97	103.83	113.06
2	A	581	GSH	O2-C2-N3	-2.85	116.95	122.98
2	D	314	GSH	OE1-CD1-CG1	2.84	127.17	122.02
2	D	314	GSH	O2-C2-CA2	2.60	125.93	120.48
2	A	581	GSH	CG1-CB1-CA1	-2.41	108.34	113.86
2	A	581	GSH	CB2-CA2-N2	-2.36	107.91	111.28

There are no chirality outliers.

All (12) 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	O11-C1-CA1-N1
2	A	581	GSH	O2-C2-CA2-N2
2	D	314	GSH	O2-C2-CA2-N2
2	A	581	GSH	N3-C2-CA2-N2
2	A	581	GSH	O12-C1-CA1-N1
2	D	314	GSH	O11-C1-CA1-N1
2	D	314	GSH	N3-C2-CA2-N2
2	A	581	GSH	O12-C1-CA1-CB1
2	A	581	GSH	O11-C1-CA1-CB1
2	A	581	GSH	O2-C2-CA2-CB2

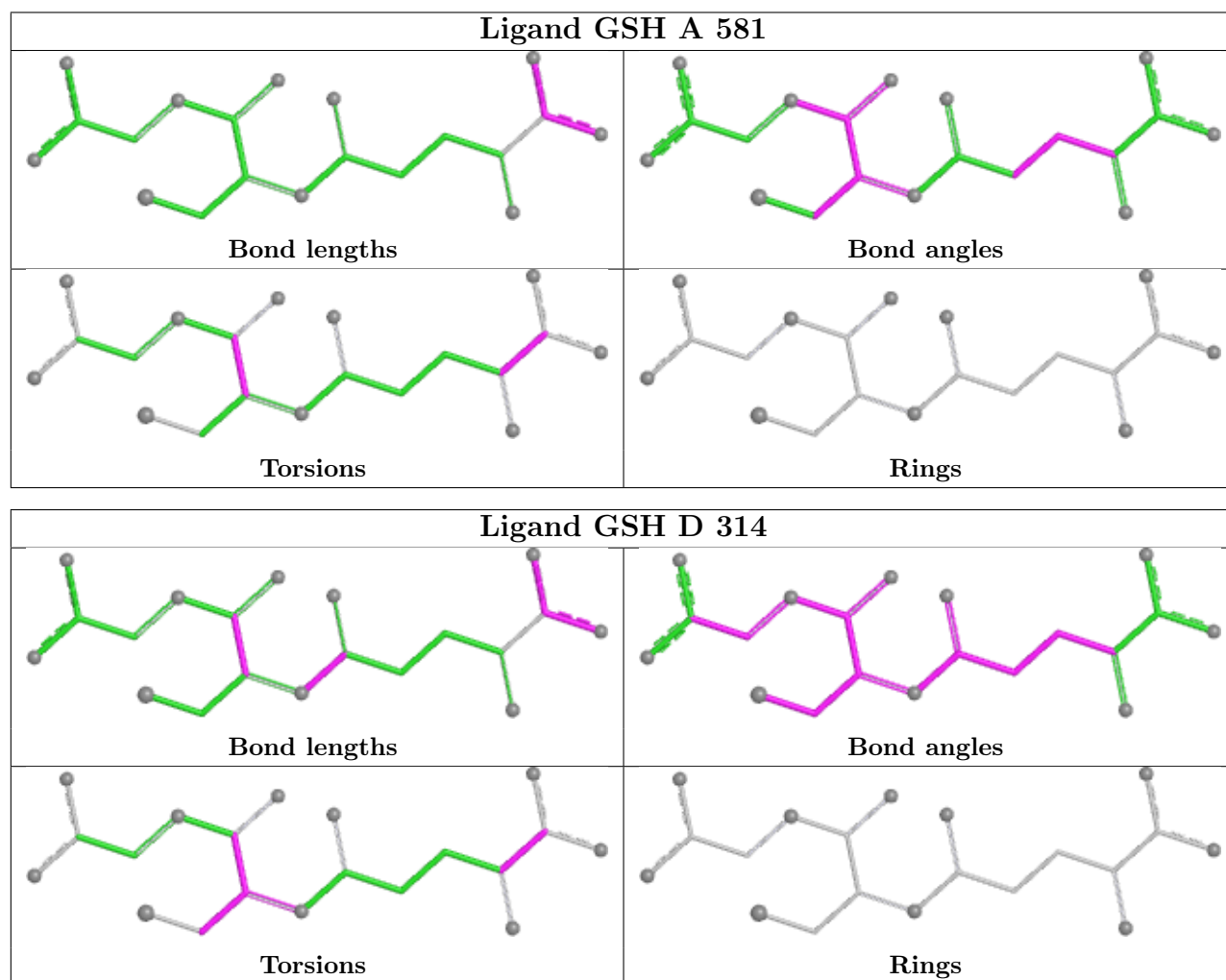
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	314	GSH	11	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	281/313 (89%)	-0.00	1 (0%) 88 89	40, 65, 98, 114	0
1	B	281/313 (89%)	0.37	10 (3%) 46 44	42, 83, 126, 142	0
1	C	280/313 (89%)	0.44	9 (3%) 50 48	42, 83, 128, 153	0
1	D	281/313 (89%)	0.97	30 (10%) 11 10	49, 110, 137, 159	0
1	E	280/313 (89%)	1.03	34 (12%) 8 7	54, 110, 154, 165	0
All	All	1403/1565 (89%)	0.56	84 (5%) 27 28	40, 88, 136, 165	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	305	PRO	3.7
1	D	153	TYR	3.5
1	E	300	GLY	3.4
1	D	204	VAL	3.3
1	D	185	ARG	3.3
1	D	298	ILE	3.2
1	D	137	PHE	3.1
1	D	202	TYR	3.0
1	D	282	LEU	3.0
1	D	288	ILE	3.0
1	D	297	GLN	2.9
1	E	95	SER	2.9
1	E	108	ILE	2.8
1	E	191	ALA	2.8
1	E	58	VAL	2.8
1	C	281	ILE	2.7
1	D	276	PHE	2.7
1	E	123	PHE	2.7
1	E	47	LYS	2.7
1	C	79	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	293	ALA	2.7
1	D	89	LEU	2.7
1	E	215	ARG	2.7
1	D	142	PHE	2.7
1	E	29	GLY	2.6
1	E	189	LEU	2.6
1	D	203	VAL	2.6
1	D	277	PRO	2.6
1	E	26	PRO	2.6
1	D	184	PRO	2.6
1	E	111	ALA	2.6
1	E	257	ILE	2.6
1	C	74	LEU	2.5
1	A	26	PRO	2.5
1	D	296	PHE	2.5
1	E	267	ILE	2.5
1	E	74	LEU	2.5
1	D	161	LEU	2.5
1	E	72	PRO	2.5
1	E	126	ARG	2.5
1	D	139	TRP	2.5
1	B	26	PRO	2.5
1	C	277	PRO	2.4
1	D	92	ILE	2.4
1	E	109	TRP	2.4
1	E	127	GLU	2.4
1	E	301	TYR	2.4
1	B	123	PHE	2.4
1	B	126	ARG	2.4
1	D	275	PRO	2.4
1	B	147	ARG	2.4
1	D	197	ALA	2.4
1	C	276	PHE	2.3
1	E	192	LEU	2.3
1	D	168	ILE	2.3
1	E	153	TYR	2.3
1	D	131	LEU	2.3
1	B	77	LYS	2.2
1	E	144	ALA	2.2
1	B	286	GLU	2.2
1	E	129	GLY	2.2
1	B	125	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	194	PRO	2.2
1	D	73	LEU	2.2
1	D	74	LEU	2.2
1	C	112	ASN	2.1
1	D	120	SER	2.1
1	E	197	ALA	2.1
1	D	306	THR	2.1
1	E	35	GLY	2.1
1	B	128	GLU	2.1
1	C	280	ARG	2.1
1	C	75	THR	2.1
1	E	273	PRO	2.1
1	E	221	LEU	2.1
1	E	252	LEU	2.1
1	B	113	GLY	2.1
1	E	254	ASP	2.1
1	E	44	GLY	2.1
1	D	96	THR	2.0
1	C	305	PRO	2.0
1	D	300	GLY	2.0
1	B	114	SER	2.0
1	E	34	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

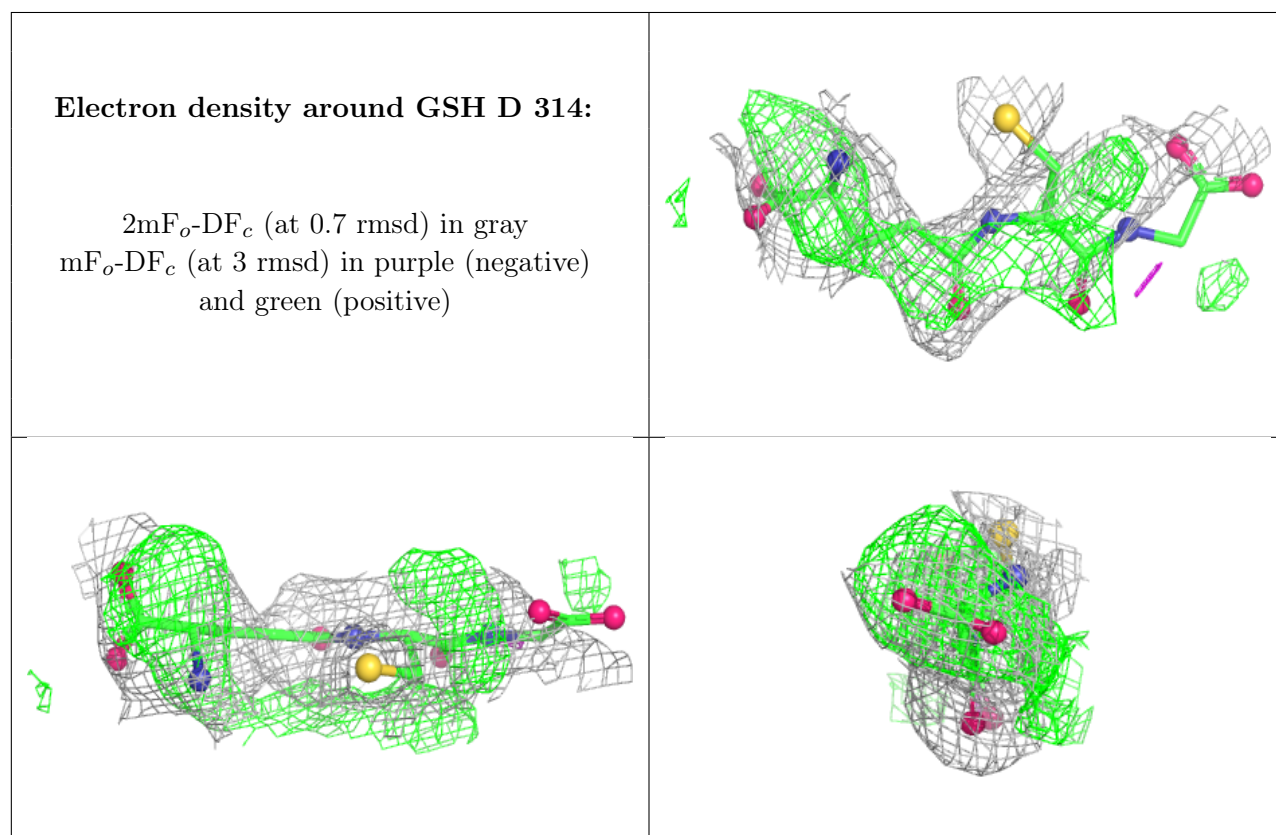
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	E	366	5/5	0.73	0.16	148,150,151,152	0

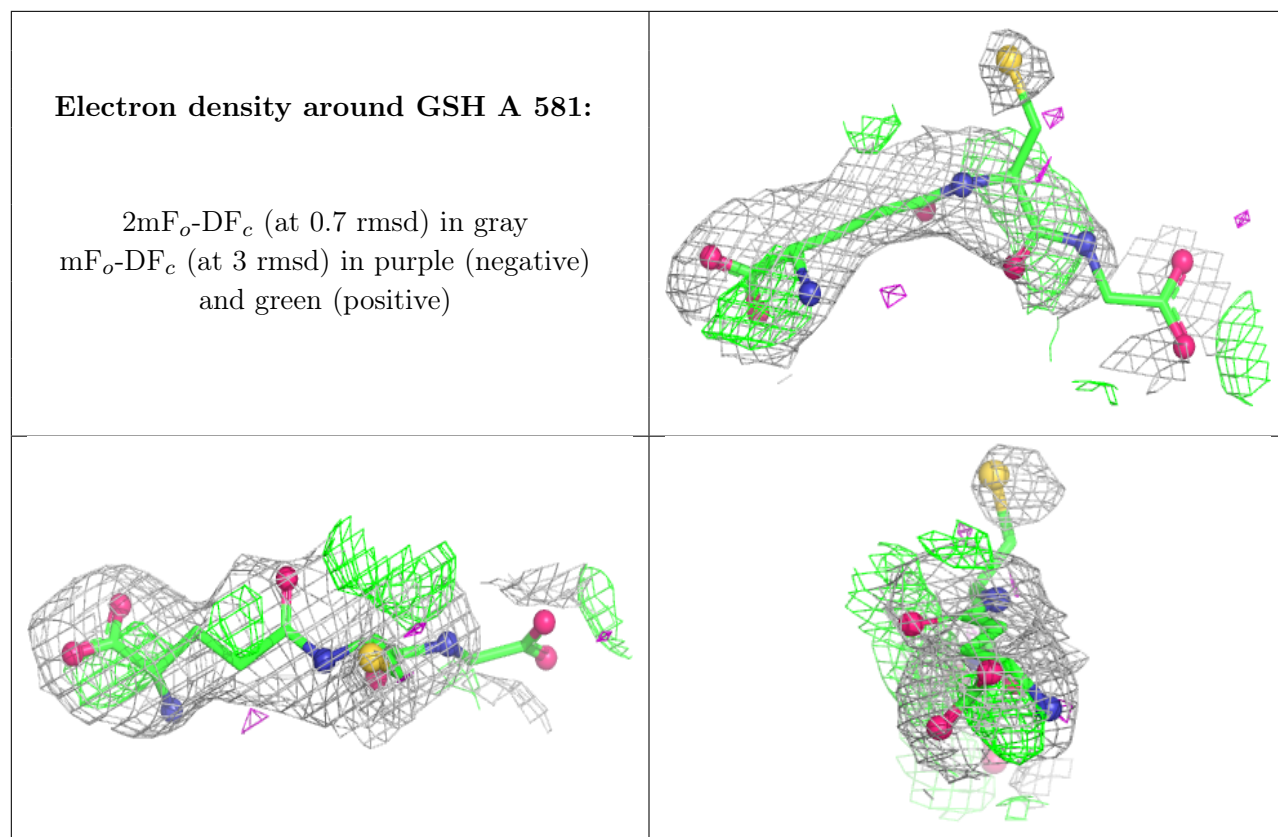
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GSH	D	314	20/20	0.75	0.30	63,102,125,128	20
2	GSH	A	581	20/20	0.80	0.24	46,118,153,154	0
3	PO4	C	365	5/5	0.81	0.12	118,119,120,122	0
3	PO4	A	365	5/5	0.93	0.11	87,89,90,94	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.