



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:17 am BST

PDB ID : 4I9U
Title : Crystal structure of rabbit LDHA in complex with a fragment inhibitor AP26256
Authors : Zhou, T.; Kohlmann, A.; Stephan, Z.G.; Commodore, L.; Greenfield, M.T.; Zhu, X.; Dalgarno, D.C.
Deposited on : 2012-12-05
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

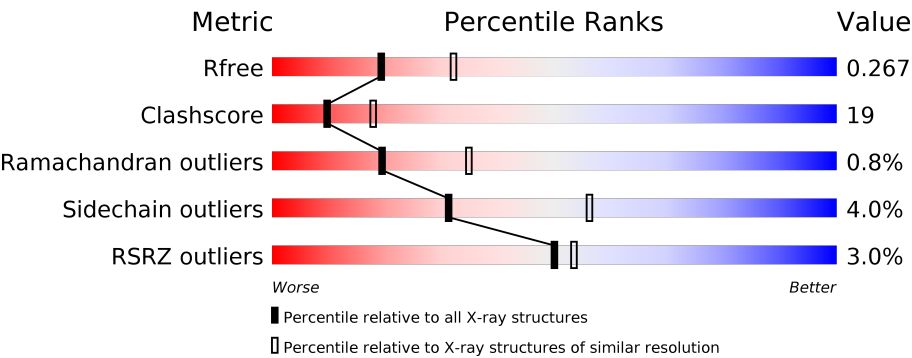
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	331	<div><div>2%</div><div><div></div><div>66%</div><div>27%</div><div></div></div><div></div></div>
1	B	331	<div><div>5%</div><div><div></div><div>64%</div><div>30%</div><div></div></div><div></div></div>
1	C	331	<div><div>3%</div><div><div></div><div>65%</div><div>34%</div><div></div></div><div></div></div>
1	D	331	<div><div>2%</div><div><div></div><div>65%</div><div>34%</div><div></div></div><div></div></div>
1	E	331	<div><div>3%</div><div><div></div><div>63%</div><div>34%</div><div></div></div><div></div></div>
1	F	331	<div><div>3%</div><div><div></div><div>62%</div><div>34%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	331	<div><div></div><div>4%</div><div>59%</div><div>36%</div><div></div><div></div></div>
1	H	331	<div><div></div><div>2%</div><div>59%</div><div>36%</div><div></div><div></div></div>

2 Entry composition

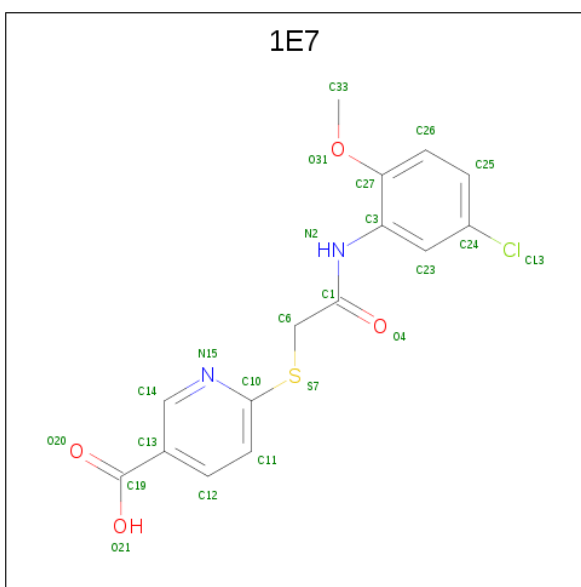
There are 3 unique types of molecules in this entry. The entry contains 20734 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2494	1596	428	456	14			
1	B	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	C	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	D	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	E	331	Total	C	N	O	S	0	0	0
			2559	1633	441	471	14			
1	F	329	Total	C	N	O	S	0	0	0
			2540	1622	437	467	14			
1	G	326	Total	C	N	O	S	0	0	0
			2517	1610	431	462	14			
1	H	326	Total	C	N	O	S	0	0	0
			2517	1610	431	462	14			

- Molecule 2 is 6-({2-[(5-chloro-2-methoxyphenyl)amino]-2-oxoethyl}sulfanyl)pyridine-3-carboxylic acid (three-letter code: 1E7) (formula: C₁₅H₁₃ClN₂O₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 23	C 15	Cl 1	N 2	O 4	S 1	0	0
2	B	1	Total 23	C 15	Cl 1	N 2	O 4	S 1	0	0
2	C	1	Total 23	C 15	Cl 1	N 2	O 4	S 1	0	0
2	D	1	Total 23	C 15	Cl 1	N 2	O 4	S 1	0	0
2	E	1	Total 23	C 15	Cl 1	N 2	O 4	S 1	0	0
2	F	1	Total 23	C 15	Cl 1	N 2	O 4	S 1	0	0
2	G	1	Total 23	C 15	Cl 1	N 2	O 4	S 1	0	0
2	H	1	Total 23	C 15	Cl 1	N 2	O 4	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		
3	B	47	Total	O	0	0
			47	47		
3	C	25	Total	O	0	0
			25	25		
3	D	31	Total	O	0	0
			31	31		

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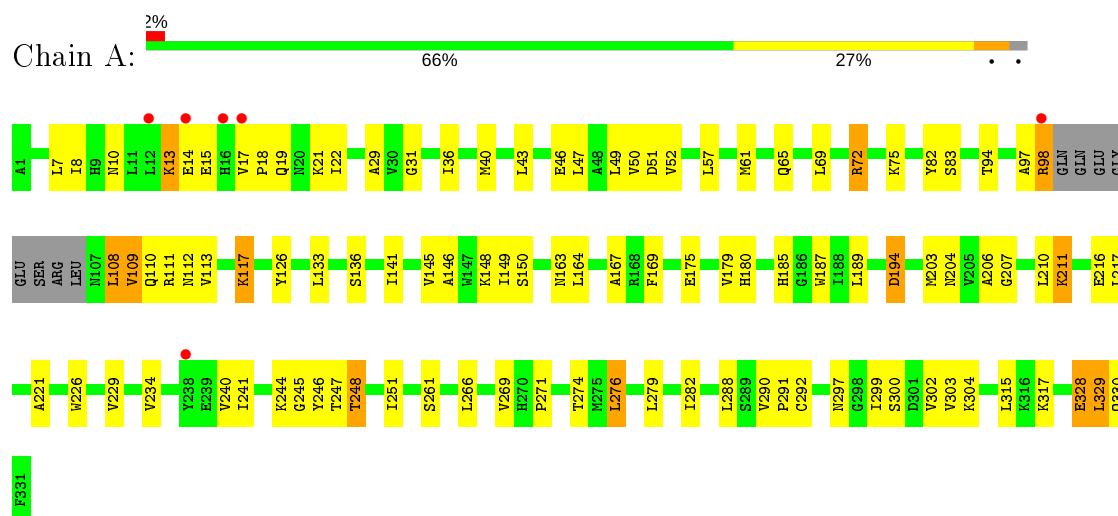
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	17	Total 17	O 17	0	0
3	F	27	Total 27	O 27	0	0
3	G	26	Total 26	O 26	0	0
3	H	33	Total 33	O 33	0	0

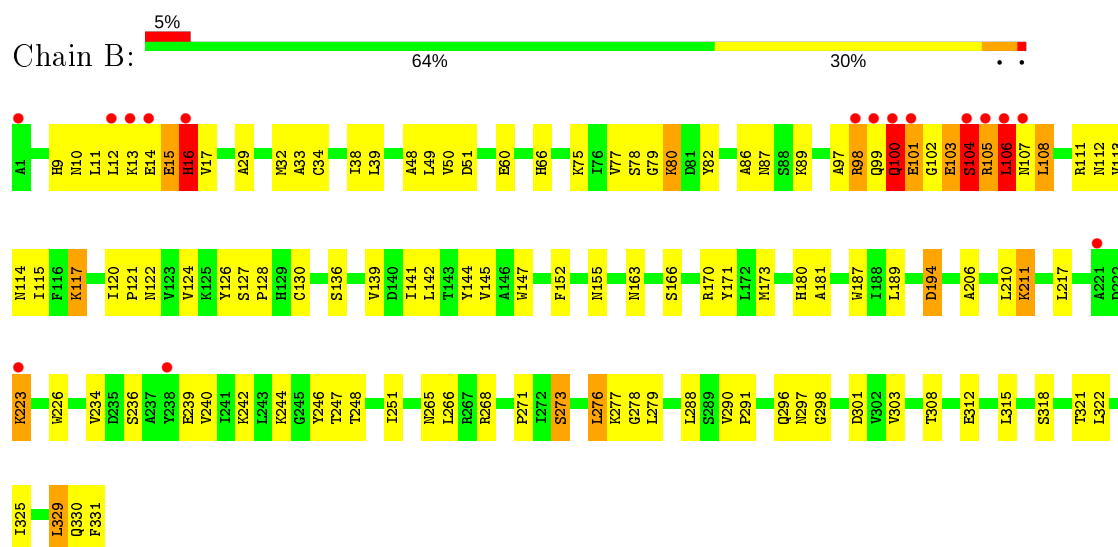
3 Residue-property plots

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

• Molecule 1: L-lactate dehydrogenase A chain

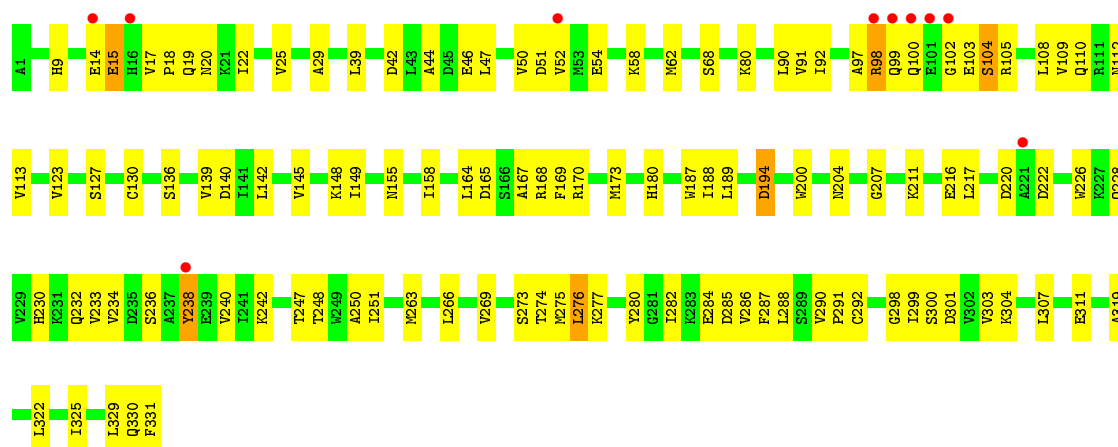


• Molecule 1: L-lactate dehydrogenase A chain

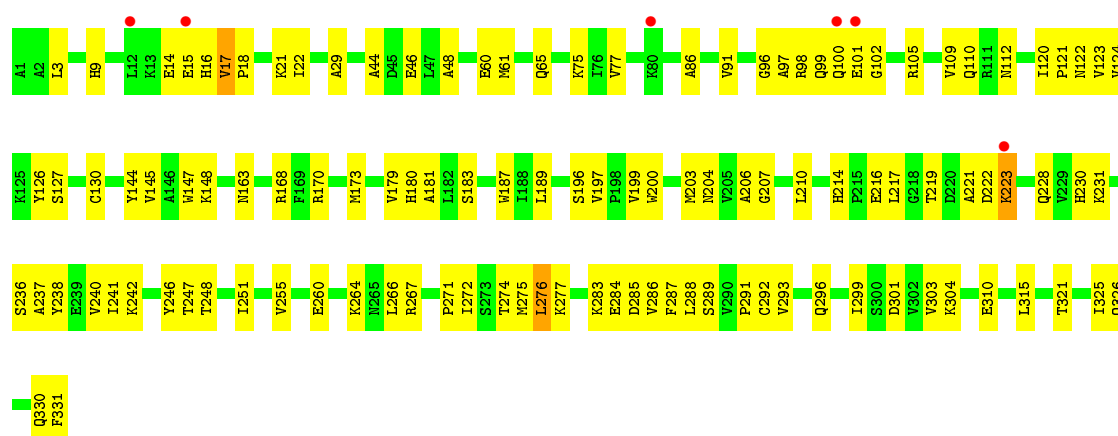


• Molecule 1: L-lactate dehydrogenase A chain

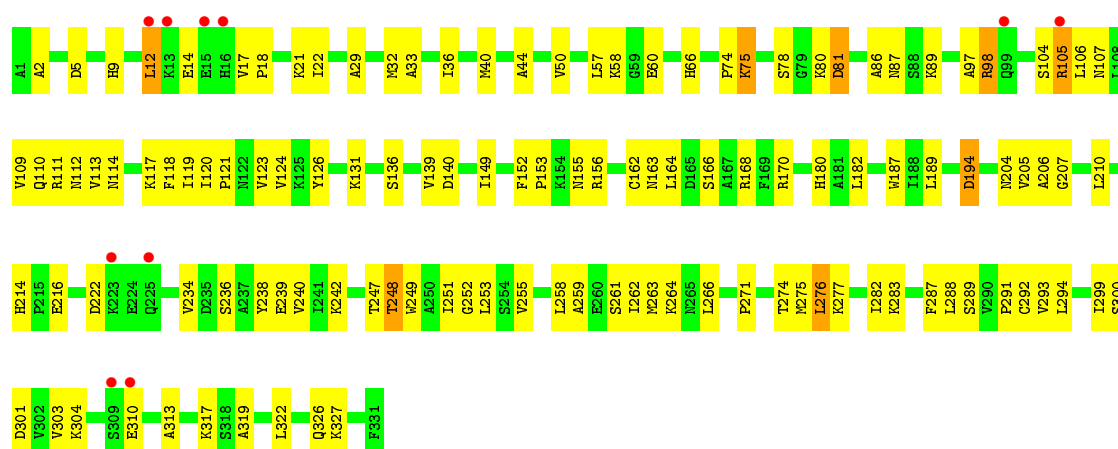




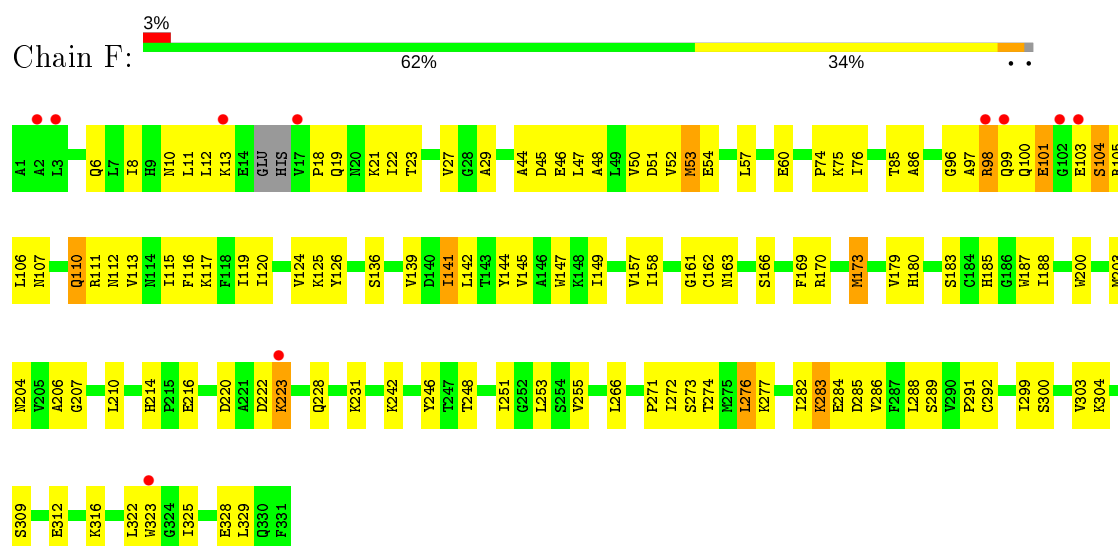
• Molecule 1: L-lactate dehydrogenase A chain



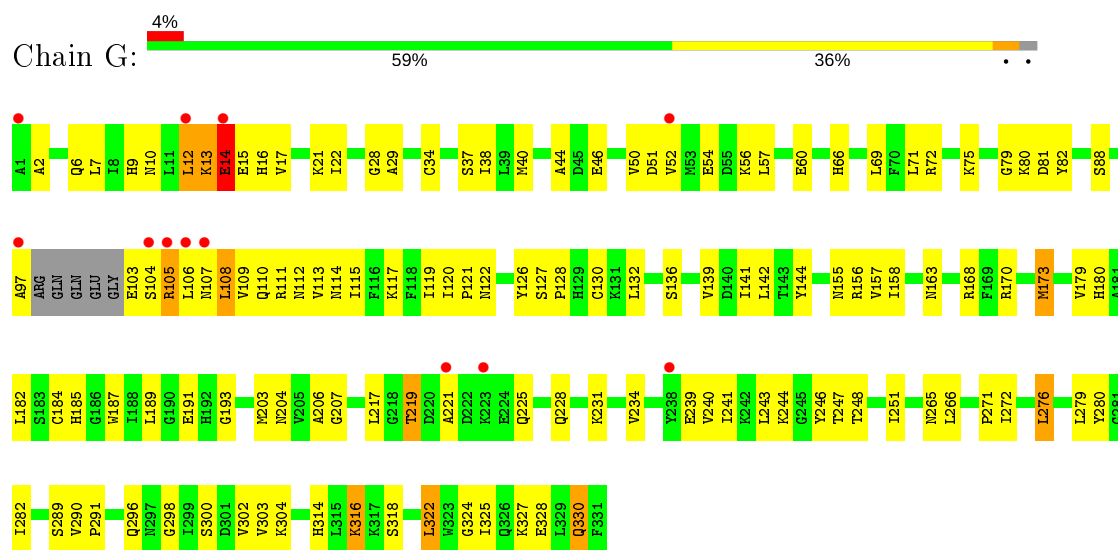
• Molecule 1: L-lactate dehydrogenase A chain



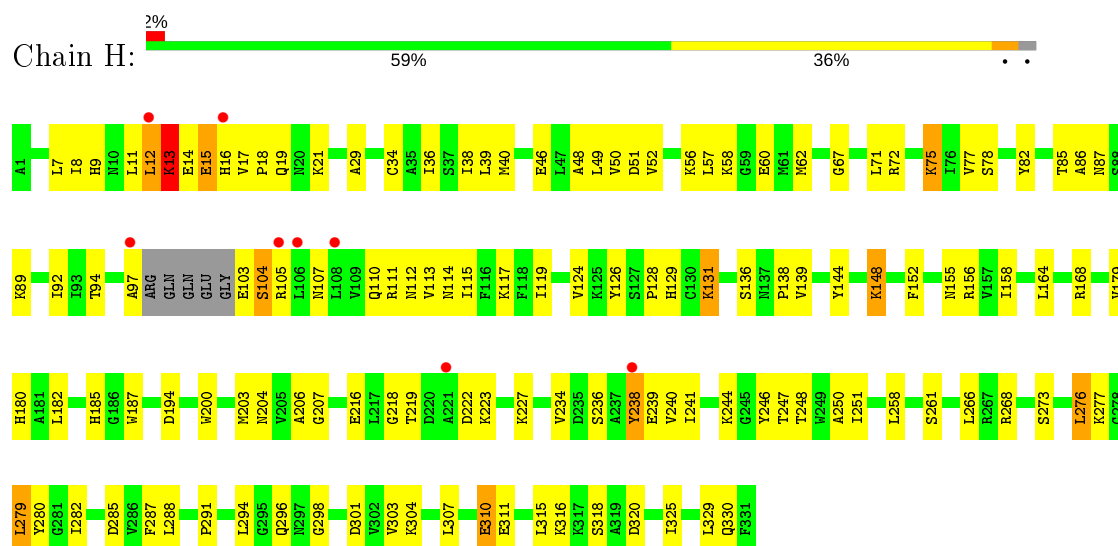
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.69Å 138.74Å 138.17Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 48.86 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (50.00-2.50) 95.9 (48.86-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.273 0.215 , 0.267	Depositor DCC
R_{free} test set	5398 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20734	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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: 1E7

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/2539	0.58	2/3434 (0.1%)
1	B	0.38	0/2605	0.54	0/3523
1	C	0.35	0/2605	0.54	0/3523
1	D	0.37	0/2605	0.54	0/3523
1	E	0.33	0/2605	0.52	0/3523
1	F	0.33	0/2584	0.52	0/3493
1	G	0.34	0/2562	0.53	0/3465
1	H	0.35	0/2562	0.54	0/3465
All	All	0.35	0/20667	0.54	2/27949 (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	A	0	1
1	B	0	3
1	H	0	1
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	LEU	CB-CG-CD1	-9.09	95.54	111.00
1	A	108	LEU	CA-CB-CG	5.20	127.26	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	LYS	Peptide
1	B	104	SER	Peptide
1	B	15	GLU	Peptide
1	B	16	HIS	Peptide
1	H	15	GLU	Peptide

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	2494	0	2578	80	0
1	B	2559	0	2639	123	0
1	C	2559	0	2639	91	0
1	D	2559	0	2639	112	0
1	E	2559	0	2639	112	0
1	F	2540	0	2625	116	0
1	G	2517	0	2600	119	0
1	H	2517	0	2600	113	0
2	A	23	0	12	0	0
2	B	23	0	12	1	0
2	C	23	0	12	1	0
2	D	23	0	12	0	0
2	E	23	0	12	1	0
2	F	23	0	12	0	0
2	G	23	0	12	1	0
2	H	23	0	12	1	0
3	A	40	0	0	1	0
3	B	47	0	0	2	0
3	C	25	0	0	2	0
3	D	31	0	0	1	0
3	E	17	0	0	2	0
3	F	27	0	0	1	0
3	G	26	0	0	0	0
3	H	33	0	0	1	0
All	All	20734	0	21055	800	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 19.

All (800) 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:276:LEU:HD21	1:D:288:LEU:HD12	1.34	1.05
1:G:219:THR:HG23	1:G:221:ALA:H	1.15	1.03
1:E:9:HIS:HB2	1:F:304:LYS:HD2	1.39	1.01
1:F:276:LEU:HD21	1:F:282:ILE:HD12	1.40	0.98
1:B:97:ALA:H	1:B:112:ASN:HD21	1.06	0.97
1:G:29:ALA:HB1	1:G:248:THR:CG2	1.95	0.95
1:G:29:ALA:HB1	1:G:248:THR:HG22	1.50	0.93
1:B:223:LYS:HD2	1:B:223:LYS:H	1.33	0.93
1:G:300:SER:HA	1:H:12:LEU:HB2	1.52	0.92
1:B:12:LEU:HG	1:B:14:GLU:HB2	1.51	0.90
1:B:14:GLU:HG3	1:B:15:GLU:H	1.33	0.90
1:A:304:LYS:HD2	1:B:9:HIS:HB2	1.53	0.90
1:B:98:ARG:HH11	1:B:98:ARG:HG2	1.36	0.90
1:E:98:ARG:H	1:E:98:ARG:HE	1.18	0.89
1:D:101:GLU:OE1	1:D:102:GLY:HA3	1.71	0.88
1:H:29:ALA:HB1	1:H:248:THR:HG21	1.54	0.86
1:A:97:ALA:H	1:A:112:ASN:HD21	1.21	0.86
1:D:29:ALA:HB1	1:D:248:THR:HG21	1.56	0.86
1:E:236:SER:O	1:E:240:VAL:HG23	1.76	0.86
1:B:29:ALA:HB1	1:B:248:THR:CG2	2.06	0.85
1:B:97:ALA:H	1:B:112:ASN:ND2	1.75	0.84
1:F:29:ALA:HB1	1:F:248:THR:HG21	1.60	0.84
1:G:219:THR:HG23	1:G:221:ALA:N	1.94	0.83
1:F:29:ALA:HB1	1:F:248:THR:CG2	2.09	0.83
1:A:29:ALA:HB1	1:A:248:THR:HG21	1.62	0.81
1:B:98:ARG:HH11	1:B:98:ARG:CG	1.93	0.81
1:G:97:ALA:H	1:G:112:ASN:ND2	1.78	0.81
1:E:29:ALA:HB1	1:E:248:THR:CG2	2.12	0.80
1:H:291:PRO:HB2	1:H:303:VAL:HB	1.64	0.80
1:A:46:GLU:OE1	1:A:75:LYS:HD3	1.82	0.79
1:E:163:ASN:HA	1:E:271:PRO:HG2	1.64	0.79
1:E:204:ASN:HD22	1:E:207:GLY:H	1.31	0.79
1:H:131:LYS:HE3	1:H:296:GLN:O	1.83	0.79
1:H:12:LEU:C	1:H:13:LYS:HG3	2.04	0.78
1:E:97:ALA:H	1:E:112:ASN:HD21	1.32	0.78
1:E:98:ARG:N	1:E:98:ARG:HE	1.80	0.78
1:G:97:ALA:H	1:G:112:ASN:HD21	1.31	0.78
1:H:310:GLU:HG3	1:H:311:GLU:N	1.99	0.77
1:A:29:ALA:HB1	1:A:248:THR:CG2	2.15	0.76
1:F:276:LEU:CD2	1:F:282:ILE:HD12	2.14	0.76
1:F:139:VAL:HG21	1:F:161:GLY:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:H	1:C:112:ASN:HD21	1.33	0.76
1:D:277:LYS:HE3	1:D:283:LYS:O	1.85	0.76
1:B:97:ALA:N	1:B:112:ASN:HD21	1.84	0.76
1:B:14:GLU:HG3	1:B:15:GLU:N	2.01	0.75
1:H:57:LEU:HG	1:H:78:SER:HB2	1.69	0.75
1:G:9:HIS:HB2	1:H:304:LYS:HD2	1.68	0.75
1:F:104:SER:HA	1:F:107:ASN:HB2	1.68	0.75
1:B:98:ARG:NH1	1:B:98:ARG:HG2	1.94	0.75
1:B:101:GLU:HG3	1:B:102:GLY:H	1.50	0.74
1:B:240:VAL:CG1	1:B:247:THR:HG22	2.17	0.74
1:F:18:PRO:HB3	1:F:46:GLU:OE1	1.88	0.74
1:D:97:ALA:H	1:D:112:ASN:HD21	1.36	0.74
1:D:101:GLU:HB2	1:D:102:GLY:CA	2.18	0.73
1:G:14:GLU:O	1:G:15:GLU:HG3	1.88	0.73
1:H:97:ALA:H	1:H:112:ASN:HD21	1.36	0.73
1:H:12:LEU:HD23	1:H:13:LYS:HE2	1.71	0.73
1:G:105:ARG:HE	1:G:325:ILE:HD13	1.53	0.73
1:C:276:LEU:HD21	1:C:288:LEU:HD12	1.70	0.72
1:E:113:VAL:O	1:E:117:LYS:HG3	1.89	0.71
1:D:145:VAL:HG13	1:D:331:PHE:HE2	1.54	0.71
1:B:101:GLU:HG3	1:B:102:GLY:N	2.06	0.71
1:C:304:LYS:HD2	1:D:9:HIS:HB2	1.73	0.71
1:D:144:TYR:CZ	1:D:148:LYS:HD2	2.26	0.71
1:A:248:THR:O	1:A:251:ILE:HG22	1.91	0.70
1:E:291:PRO:HB2	1:E:303:VAL:HB	1.72	0.70
1:C:29:ALA:HB1	1:C:248:THR:HG21	1.74	0.70
1:B:127:SER:HB3	1:B:130:CYS:HB3	1.74	0.70
1:F:285:ASP:HB2	1:F:323:TRP:HZ3	1.57	0.69
1:B:106:LEU:HD23	1:B:106:LEU:H	1.57	0.69
1:E:276:LEU:H	1:E:276:LEU:HD12	1.57	0.69
1:A:194:ASP:HA	1:A:234:VAL:HG11	1.73	0.69
1:C:29:ALA:HB1	1:C:248:THR:CG2	2.23	0.69
1:A:279:LEU:HD13	1:A:302:VAL:HG21	1.73	0.69
1:E:238:TYR:CE2	1:E:242:LYS:HE2	2.28	0.69
1:B:104:SER:O	1:B:106:LEU:N	2.26	0.69
1:B:108:LEU:HD22	1:B:108:LEU:O	1.91	0.69
1:G:187:TRP:CZ3	1:G:271:PRO:HD3	2.28	0.68
1:G:97:ALA:N	1:G:112:ASN:HD21	1.91	0.68
1:B:103:GLU:O	1:B:105:ARG:N	2.26	0.68
1:G:248:THR:O	1:G:251:ILE:HG23	1.94	0.68
1:G:276:LEU:H	1:G:276:LEU:HD12	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:VAL:HG21	1:H:329:LEU:HG	1.76	0.68
1:F:98:ARG:NH2	1:F:98:ARG:HG2	2.09	0.67
1:A:72:ARG:HH21	1:B:268:ARG:NH2	1.92	0.67
1:G:241:ILE:HG12	1:G:246:TYR:HA	1.76	0.67
1:B:51:ASP:HA	2:B:401:1E7:CL3	2.32	0.67
1:E:105:ARG:O	1:E:109:VAL:HG23	1.94	0.67
1:F:21:LYS:HD2	1:F:46:GLU:OE1	1.93	0.67
1:H:194:ASP:HA	1:H:234:VAL:HG11	1.77	0.67
1:B:29:ALA:HB1	1:B:248:THR:HG21	1.76	0.66
1:D:163:ASN:HA	1:D:271:PRO:HG2	1.75	0.66
1:H:110:GLN:HE22	1:H:330:GLN:H	1.42	0.66
1:A:204:ASN:HA	1:A:210:LEU:HD13	1.76	0.66
1:E:266:LEU:O	1:H:180:HIS:HB2	1.96	0.66
1:B:265:ASN:OD1	1:B:296:GLN:HG2	1.95	0.66
1:F:292:CYS:HB3	1:F:299:ILE:HG23	1.77	0.66
1:G:29:ALA:HB1	1:G:248:THR:HG21	1.76	0.65
1:F:98:ARG:HH21	1:F:98:ARG:HG2	1.59	0.65
1:H:261:SER:HA	1:H:266:LEU:HD12	1.78	0.65
1:H:46:GLU:OE1	1:H:75:LYS:HD2	1.96	0.65
1:B:240:VAL:HG11	1:B:247:THR:HG22	1.77	0.65
1:F:111:ARG:O	1:F:115:ILE:HG13	1.96	0.65
1:H:131:LYS:N	1:H:131:LYS:HD3	2.11	0.65
1:E:168:ARG:HE	1:G:66:HIS:CG	2.13	0.65
1:B:113:VAL:HG21	1:B:329:LEU:HG	1.79	0.65
1:C:204:ASN:HD22	1:C:207:GLY:H	1.44	0.65
1:G:324:GLY:HA2	1:G:327:LYS:HE2	1.78	0.65
1:D:276:LEU:HD12	1:D:286:VAL:O	1.97	0.64
1:D:22:ILE:HG13	1:D:44:ALA:HB2	1.79	0.64
1:E:97:ALA:H	1:E:112:ASN:ND2	1.93	0.64
1:B:103:GLU:OE1	1:B:105:ARG:HA	1.97	0.64
1:D:97:ALA:H	1:D:112:ASN:ND2	1.94	0.64
1:H:115:ILE:HG22	1:H:119:ILE:HD12	1.78	0.64
1:B:223:LYS:HD2	1:B:223:LYS:N	2.11	0.64
1:F:204:ASN:HD22	1:F:207:GLY:H	1.44	0.64
1:H:82:TYR:O	1:H:85:THR:HB	1.97	0.64
1:C:228:GLN:HA	1:C:228:GLN:NE2	2.10	0.64
1:F:170:ARG:HA	1:F:173:MET:HE3	1.80	0.64
1:F:277:LYS:HB2	1:F:284:GLU:O	1.98	0.64
1:H:112:ASN:HD22	1:H:115:ILE:HD12	1.63	0.64
1:C:99:GLN:HG2	1:C:100:GLN:O	1.98	0.64
1:E:282:ILE:HD12	1:E:319:ALA:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:HA	1:D:187:TRP:CZ2	2.33	0.64
1:G:302:VAL:HG13	1:H:11:LEU:HD12	1.80	0.64
1:H:104:SER:HB3	1:H:107:ASN:HB2	1.79	0.63
1:F:139:VAL:HG11	1:F:161:GLY:HA2	1.79	0.63
1:G:82:TYR:OH	1:G:119:ILE:HG23	1.98	0.63
1:A:18:PRO:HB2	1:A:21:LYS:HB2	1.79	0.63
1:B:100:GLN:O	1:B:101:GLU:HB2	1.99	0.63
1:C:42:ASP:HB3	1:D:264:LYS:HZ1	1.64	0.63
1:C:164:LEU:HD22	1:C:251:ILE:HA	1.81	0.63
1:E:276:LEU:HD21	1:E:288:LEU:HD12	1.80	0.63
1:H:105:ARG:HH22	1:H:138:PRO:HB3	1.63	0.62
1:B:170:ARG:HA	1:B:173:MET:CE	2.29	0.62
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.80	0.62
1:D:101:GLU:HB2	1:D:102:GLY:HA3	1.79	0.62
1:A:97:ALA:N	1:A:112:ASN:HD21	1.96	0.62
1:E:214:HIS:CE1	1:E:216:GLU:HB2	2.35	0.62
1:G:170:ARG:HA	1:G:173:MET:HE3	1.80	0.62
1:A:163:ASN:HA	1:A:271:PRO:HG2	1.81	0.62
1:C:228:GLN:O	1:C:232:GLN:HG3	2.00	0.62
1:G:302:VAL:HG13	1:H:11:LEU:CD1	2.30	0.62
1:B:163:ASN:HA	1:B:271:PRO:HG2	1.80	0.62
1:E:17:VAL:O	1:E:17:VAL:HG23	2.00	0.62
1:H:136:SER:O	1:H:139:VAL:HA	2.00	0.62
1:D:16:HIS:CE1	1:D:75:LYS:HD2	2.34	0.62
1:C:275:MET:HG2	1:C:287:PHE:CE2	2.35	0.62
1:C:58:LYS:O	1:C:62:MET:HG3	1.99	0.62
1:F:277:LYS:HD3	1:F:285:ASP:OD2	1.99	0.61
1:G:110:GLN:HA	1:G:113:VAL:HB	1.81	0.61
1:D:274:THR:HB	1:D:299:ILE:HD13	1.81	0.61
1:D:100:GLN:HB3	1:D:101:GLU:CD	2.19	0.61
1:C:15:GLU:O	1:C:17:VAL:HG23	2.00	0.61
1:D:101:GLU:CB	1:D:102:GLY:HA3	2.30	0.61
1:B:106:LEU:H	1:B:106:LEU:CD2	2.13	0.61
1:C:286:VAL:HG13	1:C:322:LEU:HD23	1.83	0.60
1:D:204:ASN:HD22	1:D:207:GLY:H	1.48	0.60
1:H:71:LEU:O	1:H:72:ARG:HD2	2.01	0.60
1:B:145:VAL:HG13	1:B:331:PHE:HE2	1.66	0.60
1:D:240:VAL:HG11	1:D:247:THR:HG22	1.83	0.60
1:E:89:LYS:HE3	3:E:505:HOH:O	2.00	0.60
1:A:17:VAL:O	1:A:17:VAL:HG13	2.02	0.60
1:E:98:ARG:H	1:E:98:ARG:NE	1.96	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:16:HIS:NE2	1:G:46:GLU:OE1	2.31	0.60
1:G:304:LYS:HD2	1:H:9:HIS:HB2	1.83	0.60
1:D:223:LYS:HD2	1:D:223:LYS:H	1.65	0.60
1:F:51:ASP:H	1:F:57:LEU:HD22	1.67	0.60
1:G:141:ILE:HD11	1:G:322:LEU:HD12	1.84	0.60
1:C:110:GLN:HE22	1:C:330:GLN:H	1.49	0.60
1:F:98:ARG:HH21	1:F:98:ARG:CG	2.14	0.60
1:G:108:LEU:O	1:G:108:LEU:HD12	2.01	0.60
1:B:105:ARG:O	1:B:107:ASN:N	2.33	0.60
1:B:80:LYS:NZ	1:B:80:LYS:HB3	2.16	0.60
1:F:158:ILE:CG2	1:F:272:ILE:HD12	2.32	0.59
1:A:241:ILE:HG23	1:A:245:GLY:O	2.03	0.59
1:A:36:ILE:O	1:A:40:MET:HG3	2.02	0.59
1:E:66:HIS:HB3	1:G:168:ARG:HG2	1.83	0.59
1:A:328:GLU:O	1:A:329:LEU:O	2.20	0.59
1:A:61:MET:O	1:A:65:GLN:HG3	2.03	0.59
1:C:277:LYS:HD3	1:C:285:ASP:OD2	2.02	0.59
1:F:98:ARG:NE	1:F:98:ARG:H	2.00	0.59
1:D:144:TYR:OH	1:D:148:LYS:HD2	2.03	0.59
1:H:103:GLU:O	1:H:104:SER:HB3	2.03	0.59
1:F:210:LEU:HD21	1:H:7:LEU:HD22	1.84	0.59
1:C:291:PRO:HB2	1:C:303:VAL:HB	1.85	0.59
1:D:170:ARG:HA	1:D:173:MET:HE3	1.85	0.59
1:D:219:THR:HG22	1:D:222:ASP:HB2	1.85	0.59
1:D:29:ALA:HB1	1:D:248:THR:CG2	2.31	0.59
1:G:105:ARG:HE	1:G:325:ILE:CD1	2.15	0.59
1:F:115:ILE:O	1:F:119:ILE:HG13	2.03	0.58
1:D:292:CYS:HB3	1:D:299:ILE:HG23	1.83	0.58
1:G:136:SER:O	1:G:142:LEU:HD12	2.02	0.58
1:C:42:ASP:HB3	1:D:264:LYS:NZ	2.17	0.58
1:E:2:ALA:HB3	1:E:5:ASP:OD1	2.03	0.58
1:H:164:LEU:HD11	1:H:250:ALA:HB1	1.85	0.58
1:A:108:LEU:O	1:A:110:GLN:N	2.36	0.58
1:C:282:ILE:HD12	1:C:319:ALA:HB2	1.86	0.58
1:A:240:VAL:CG1	1:A:247:THR:HG22	2.33	0.58
1:A:279:LEU:CD1	1:A:302:VAL:HG21	2.33	0.58
1:D:276:LEU:HD12	1:D:276:LEU:H	1.69	0.58
1:E:322:LEU:O	1:E:326:GLN:HG3	2.04	0.58
1:E:29:ALA:HB1	1:E:248:THR:HG21	1.86	0.58
1:G:204:ASN:HD22	1:G:207:GLY:H	1.51	0.58
1:G:240:VAL:HG11	1:G:247:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:HIS:O	1:F:203:MET:HA	2.04	0.58
1:E:40:MET:HE1	1:G:40:MET:HB2	1.86	0.58
1:B:273:SER:HA	1:B:288:LEU:O	2.04	0.57
1:A:175:GLU:HA	1:A:175:GLU:OE2	2.05	0.57
1:H:103:GLU:O	1:H:104:SER:CB	2.52	0.57
1:G:2:ALA:O	1:G:6:GLN:HG3	2.04	0.57
1:E:131:LYS:N	1:E:131:LYS:HD3	2.19	0.57
1:A:291:PRO:HB2	1:A:303:VAL:HB	1.86	0.57
1:C:204:ASN:ND2	1:C:207:GLY:H	2.02	0.57
1:E:251:ILE:O	1:E:255:VAL:HG23	2.05	0.57
1:H:103:GLU:N	3:H:524:HOH:O	2.37	0.57
1:G:158:ILE:HG23	1:G:272:ILE:HD12	1.85	0.57
1:G:240:VAL:CG1	1:G:247:THR:HG22	2.34	0.57
1:G:189:LEU:HD22	1:G:290:VAL:HA	1.87	0.57
1:G:71:LEU:O	1:G:72:ARG:HD3	2.04	0.57
1:H:246:TYR:CD2	1:H:248:THR:HG23	2.40	0.57
1:D:120:ILE:O	1:D:124:VAL:HG23	2.05	0.56
1:E:247:THR:O	1:E:248:THR:HG23	2.05	0.56
1:D:96:GLY:HA2	1:D:112:ASN:ND2	2.20	0.56
1:E:86:ALA:HA	1:E:126:TYR:O	2.05	0.56
1:G:291:PRO:HB2	1:G:303:VAL:HB	1.86	0.56
1:B:99:GLN:C	1:B:100:GLN:HG3	2.25	0.56
1:D:228:GLN:HE22	1:D:231:LYS:HD2	1.71	0.56
1:E:310:GLU:O	1:E:313:ALA:HB3	2.04	0.56
1:F:274:THR:HB	1:F:299:ILE:HD13	1.86	0.56
1:G:239:GLU:O	1:G:243:LEU:HG	2.06	0.56
1:H:12:LEU:HD13	1:H:14:GLU:HB2	1.87	0.56
1:H:216:GLU:O	1:H:222:ASP:HB2	2.05	0.56
1:B:103:GLU:HG3	1:B:108:LEU:HB3	1.86	0.56
1:F:27:VAL:HG13	1:F:51:ASP:HB2	1.87	0.56
1:B:101:GLU:CG	1:B:102:GLY:H	2.19	0.56
1:B:239:GLU:O	1:B:242:LYS:HB3	2.06	0.56
1:A:17:VAL:HG13	1:A:19:GLN:HE21	1.70	0.56
1:F:97:ALA:H	1:F:112:ASN:ND2	2.03	0.56
1:G:265:ASN:OD1	1:G:296:GLN:HG2	2.05	0.56
1:E:204:ASN:ND2	1:E:207:GLY:H	2.03	0.56
1:H:86:ALA:O	1:H:87:ASN:HB2	2.06	0.56
1:F:113:VAL:HG22	1:F:145:VAL:HG21	1.88	0.55
1:C:54:GLU:CD	1:C:80:LYS:HD3	2.26	0.55
1:G:29:ALA:CB	1:G:248:THR:HG22	2.31	0.55
1:H:246:TYR:HD2	1:H:248:THR:HG23	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:THR:O	1:E:251:ILE:HG22	2.06	0.55
1:G:246:TYR:CD2	1:G:248:THR:HG23	2.41	0.55
1:B:276:LEU:HD21	1:B:288:LEU:HB2	1.87	0.55
1:C:236:SER:O	1:C:240:VAL:HG23	2.06	0.55
1:D:105:ARG:O	1:D:109:VAL:HG23	2.06	0.55
1:C:20:ASN:HB3	1:C:263:MET:CE	2.37	0.55
1:G:204:ASN:ND2	1:G:207:GLY:H	2.04	0.55
1:D:15:GLU:O	1:D:15:GLU:HG3	2.06	0.55
1:C:25:VAL:HG13	1:C:50:VAL:HG23	1.89	0.55
1:H:29:ALA:HB1	1:H:248:THR:CG2	2.34	0.55
1:B:103:GLU:CG	1:B:108:LEU:HB3	2.37	0.54
1:F:276:LEU:C	1:F:276:LEU:HD13	2.27	0.54
1:D:120:ILE:HB	1:D:121:PRO:HD3	1.89	0.54
1:G:180:HIS:CE1	1:G:182:LEU:HG	2.42	0.54
1:G:51:ASP:OD1	1:G:52:VAL:N	2.37	0.54
1:A:10:ASN:HA	1:B:301:ASP:OD2	2.08	0.54
1:C:103:GLU:O	1:C:104:SER:CB	2.56	0.54
1:A:297:ASN:OD1	1:B:14:GLU:HG2	2.07	0.54
1:G:163:ASN:HA	1:G:271:PRO:HG2	1.90	0.54
1:G:46:GLU:HG3	1:G:75:LYS:HB3	1.89	0.54
1:E:206:ALA:HA	1:H:187:TRP:CZ2	2.43	0.54
1:D:122:ASN:ND2	3:D:530:HOH:O	2.40	0.54
1:H:248:THR:O	1:H:251:ILE:HG22	2.08	0.54
1:B:194:ASP:HA	1:B:234:VAL:HG11	1.89	0.54
1:C:97:ALA:H	1:C:112:ASN:ND2	2.04	0.54
1:D:127:SER:HB3	1:D:130:CYS:HB3	1.90	0.54
1:D:219:THR:HG23	1:D:221:ALA:N	2.23	0.54
1:B:210:LEU:HD22	1:D:3:LEU:HD11	1.90	0.54
1:E:170:ARG:HD3	1:G:69:LEU:HD22	1.90	0.54
1:D:97:ALA:N	1:D:112:ASN:HD21	2.04	0.54
1:D:179:VAL:CG1	1:D:183:SER:HB2	2.39	0.53
1:C:100:GLN:HB2	1:C:103:GLU:HB2	1.90	0.53
1:B:266:LEU:O	1:C:180:HIS:HB2	2.07	0.53
1:F:179:VAL:CG1	1:F:183:SER:HB2	2.38	0.53
1:H:277:LYS:HD3	1:H:285:ASP:OD2	2.07	0.53
1:B:29:ALA:HB1	1:B:248:THR:HG22	1.89	0.53
1:D:236:SER:O	1:D:240:VAL:HG23	2.08	0.53
1:D:46:GLU:OE1	1:D:75:LYS:HD3	2.08	0.53
1:E:249:TRP:O	1:E:253:LEU:HG	2.08	0.53
1:F:98:ARG:H	1:F:98:ARG:CD	2.21	0.53
1:B:187:TRP:CZ3	1:B:271:PRO:HD3	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:MET:HE1	1:B:60:GLU:HB3	1.91	0.53
1:G:265:ASN:CG	1:G:296:GLN:HG2	2.29	0.53
1:A:13:LYS:HD3	1:A:13:LYS:C	2.29	0.53
1:A:146:ALA:O	1:A:150:SER:HB3	2.08	0.53
1:C:194:ASP:HA	1:C:234:VAL:HG11	1.90	0.53
1:F:50:VAL:HG21	1:F:85:THR:HG21	1.91	0.53
1:E:109:VAL:O	1:E:113:VAL:HG23	2.09	0.53
1:E:118:PHE:O	1:E:121:PRO:HD2	2.09	0.53
1:B:279:LEU:HD22	1:B:279:LEU:N	2.24	0.53
1:D:246:TYR:CD2	1:D:248:THR:HG23	2.44	0.53
1:E:262:ILE:HG12	1:E:294:LEU:HD11	1.90	0.53
1:G:103:GLU:CD	1:G:104:SER:H	2.11	0.53
1:B:278:GLY:C	1:B:279:LEU:HD22	2.29	0.53
1:C:9:HIS:HB2	1:D:304:LYS:HD3	1.91	0.53
1:E:98:ARG:CZ	1:E:111:ARG:HH22	2.22	0.53
1:F:216:GLU:O	1:F:222:ASP:HB2	2.09	0.53
1:G:120:ILE:HB	1:G:121:PRO:HD3	1.91	0.53
1:H:258:LEU:HD22	1:H:294:LEU:HD22	1.91	0.53
1:A:276:LEU:HD21	1:A:288:LEU:HB2	1.89	0.52
1:B:246:TYR:CE2	1:B:248:THR:HG23	2.44	0.52
1:E:32:MET:HE2	1:E:60:GLU:OE1	2.08	0.52
1:C:18:PRO:HG3	1:C:46:GLU:OE1	2.09	0.52
1:C:269:VAL:HA	1:C:292:CYS:O	2.09	0.52
1:E:119:ILE:HD11	2:E:401:1E7:H8	1.91	0.52
1:G:111:ARG:HD2	2:G:401:1E7:O21	2.09	0.52
1:H:111:ARG:O	1:H:115:ILE:HG13	2.08	0.52
1:A:110:GLN:OE1	1:A:329:LEU:HA	2.10	0.52
1:B:163:ASN:HB3	3:B:543:HOH:O	2.08	0.52
1:F:141:ILE:HD13	1:F:322:LEU:HD22	1.91	0.52
1:G:57:LEU:HD21	1:G:79:GLY:H	1.75	0.52
1:B:180:HIS:HB2	1:C:266:LEU:O	2.09	0.52
1:E:98:ARG:CA	1:E:98:ARG:HE	2.18	0.52
1:F:106:LEU:HD21	1:F:328:GLU:HG3	1.91	0.52
1:F:86:ALA:HA	1:F:126:TYR:HB3	1.91	0.52
1:H:236:SER:O	1:H:240:VAL:HG23	2.10	0.52
1:F:97:ALA:H	1:F:112:ASN:HD21	1.57	0.52
1:G:155:ASN:ND2	1:G:156:ARG:HG3	2.24	0.52
1:B:101:GLU:CG	1:B:102:GLY:N	2.73	0.52
1:C:248:THR:O	1:C:251:ILE:HG22	2.10	0.52
1:D:100:GLN:NE2	1:D:100:GLN:HA	2.25	0.52
1:B:206:ALA:HA	1:C:187:TRP:CZ2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:272:ILE:O	1:G:289:SER:HA	2.10	0.51
1:C:39:LEU:HA	3:C:523:HOH:O	2.09	0.51
1:H:12:LEU:HD22	1:H:13:LYS:H	1.75	0.51
1:F:180:HIS:HB2	1:G:266:LEU:O	2.09	0.51
1:F:50:VAL:HG21	1:F:85:THR:CG2	2.40	0.51
1:B:170:ARG:HA	1:B:173:MET:HE2	1.90	0.51
1:B:210:LEU:HD13	1:D:3:LEU:HD21	1.91	0.51
1:E:194:ASP:HA	1:E:234:VAL:HG11	1.91	0.51
1:F:272:ILE:O	1:F:289:SER:HA	2.09	0.51
1:B:114:ASN:HA	1:B:117:LYS:HD3	1.93	0.51
1:E:119:ILE:O	1:E:123:VAL:HG23	2.11	0.51
1:E:274:THR:O	1:E:287:PHE:HA	2.11	0.51
1:H:144:TYR:HA	1:H:287:PHE:CE2	2.46	0.51
1:B:170:ARG:HA	1:B:173:MET:HE3	1.92	0.51
1:D:330:GLN:NE2	1:F:99:GLN:HG2	2.25	0.51
1:H:124:VAL:HG12	1:H:152:PHE:CZ	2.46	0.51
1:A:17:VAL:HG13	1:A:19:GLN:NE2	2.25	0.51
1:B:104:SER:O	1:B:106:LEU:HG	2.10	0.51
1:B:124:VAL:HG12	1:B:152:PHE:CZ	2.46	0.51
1:C:148:LYS:HE2	1:C:331:PHE:CD1	2.46	0.51
1:F:266:LEU:O	1:G:180:HIS:HB2	2.11	0.51
1:H:51:ASP:HA	2:H:401:1E7:CL3	2.48	0.51
1:E:164:LEU:HD22	1:E:251:ILE:HA	1.92	0.51
1:G:12:LEU:HD11	1:H:155:ASN:ND2	2.25	0.51
1:H:7:LEU:HG	1:H:8:ILE:HG13	1.93	0.51
1:D:246:TYR:HD2	1:D:248:THR:HG23	1.75	0.51
1:F:125:LYS:HD3	1:F:126:TYR:CE1	2.46	0.51
1:D:275:MET:HG2	1:D:287:PHE:CE2	2.46	0.50
1:F:228:GLN:HE22	1:F:231:LYS:HD3	1.76	0.50
1:F:276:LEU:HD12	1:F:286:VAL:O	2.11	0.50
1:E:301:ASP:HB3	1:F:8:ILE:HG23	1.92	0.50
1:B:246:TYR:CD2	1:B:248:THR:HG23	2.47	0.50
1:F:96:GLY:HA2	1:F:112:ASN:ND2	2.26	0.50
1:F:325:ILE:O	1:F:328:GLU:HB2	2.11	0.50
1:G:104:SER:OG	1:G:106:LEU:N	2.45	0.50
1:A:244:LYS:HE2	1:A:246:TYR:O	2.12	0.50
1:C:211:LYS:CD	1:C:217:LEU:HB3	2.41	0.50
1:E:292:CYS:HB3	1:E:299:ILE:HG23	1.94	0.50
1:G:54:GLU:OE1	1:G:80:LYS:HD3	2.11	0.50
1:H:219:THR:O	1:H:222:ASP:HB3	2.12	0.50
1:D:18:PRO:HG3	1:D:21:LYS:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ALA:O	1:D:241:ILE:HG13	2.10	0.50
1:C:127:SER:HB3	1:C:130:CYS:HB3	1.93	0.50
1:F:246:TYR:HD2	1:F:248:THR:HG23	1.77	0.50
1:H:17:VAL:O	1:H:19:GLN:NE2	2.44	0.50
1:B:120:ILE:HB	1:B:121:PRO:HD3	1.94	0.50
1:B:39:LEU:O	3:B:501:HOH:O	2.19	0.50
1:D:277:LYS:HD3	1:D:284:GLU:O	2.12	0.50
1:F:52:VAL:O	1:F:54:GLU:N	2.45	0.50
1:A:51:ASP:OD1	1:A:52:VAL:N	2.39	0.50
1:B:104:SER:O	1:B:105:ARG:C	2.49	0.50
1:E:139:VAL:HG13	1:E:140:ASP:H	1.77	0.50
1:F:163:ASN:HA	1:F:271:PRO:HG2	1.93	0.50
1:D:240:VAL:CG1	1:D:247:THR:HG22	2.42	0.50
1:E:29:ALA:HB1	1:E:248:THR:HG22	1.91	0.50
1:E:110:GLN:O	1:E:113:VAL:HB	2.11	0.50
1:E:187:TRP:CZ3	1:E:271:PRO:HD3	2.47	0.50
1:H:240:VAL:CG1	1:H:247:THR:HG22	2.42	0.50
1:C:276:LEU:CD1	1:C:282:ILE:HG21	2.42	0.49
1:A:211:LYS:HE3	1:A:217:LEU:HB3	1.94	0.49
1:H:310:GLU:HG3	1:H:311:GLU:H	1.75	0.49
1:C:280:TYR:OH	1:C:303:VAL:O	2.28	0.49
1:C:110:GLN:NE2	1:C:330:GLN:H	2.09	0.49
1:C:51:ASP:OD1	1:C:52:VAL:N	2.45	0.49
1:H:194:ASP:HA	1:H:234:VAL:CG1	2.42	0.49
1:F:204:ASN:HD22	1:F:207:GLY:N	2.09	0.49
1:F:98:ARG:NH1	1:F:111:ARG:NH2	2.60	0.49
1:A:269:VAL:HA	1:A:292:CYS:O	2.12	0.49
1:A:49:LEU:O	1:A:57:LEU:HD11	2.12	0.49
1:C:51:ASP:HA	2:C:401:1E7:CL3	2.49	0.49
1:F:179:VAL:HG12	1:F:183:SER:HB2	1.94	0.49
1:G:112:ASN:HD22	1:G:115:ILE:HD12	1.77	0.49
1:A:216:GLU:OE2	1:A:221:ALA:HB3	2.13	0.49
1:B:223:LYS:CD	1:B:223:LYS:H	2.14	0.49
1:C:273:SER:HA	1:C:288:LEU:O	2.12	0.49
1:B:226:TRP:CZ2	1:D:3:LEU:HD23	2.47	0.49
1:F:285:ASP:HB2	1:F:323:TRP:CZ3	2.42	0.49
1:G:104:SER:OG	1:G:106:LEU:HB3	2.12	0.49
1:E:282:ILE:HG23	1:E:319:ALA:HB1	1.95	0.49
1:A:15:GLU:HA	1:A:15:GLU:OE2	2.13	0.49
1:A:29:ALA:C	1:A:248:THR:HG22	2.33	0.49
1:D:260:GLU:HG2	1:D:264:LYS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:ILE:HG22	1:F:119:ILE:CD1	2.42	0.49
1:A:109:VAL:O	1:A:113:VAL:N	2.33	0.49
1:D:216:GLU:O	1:D:219:THR:HG22	2.13	0.49
1:E:32:MET:HE1	1:E:60:GLU:HB3	1.95	0.49
1:E:180:HIS:HB2	1:H:266:LEU:O	2.13	0.49
1:B:100:GLN:O	1:B:101:GLU:CB	2.61	0.48
1:B:32:MET:CE	1:B:60:GLU:HB3	2.42	0.48
1:D:210:LEU:HB3	1:D:217:LEU:HD22	1.95	0.48
1:A:247:THR:O	1:A:248:THR:HG23	2.13	0.48
1:E:259:ALA:O	1:E:263:MET:HG2	2.13	0.48
1:F:162:CYS:HB2	1:F:289:SER:CB	2.43	0.48
1:F:29:ALA:HB1	1:F:248:THR:HG22	1.91	0.48
1:H:97:ALA:H	1:H:112:ASN:ND2	2.08	0.48
1:A:7:LEU:HG	1:A:8:ILE:HG13	1.96	0.48
1:B:103:GLU:HG3	1:B:108:LEU:CB	2.43	0.48
1:C:148:LYS:HD3	1:C:331:PHE:CE2	2.48	0.48
1:C:211:LYS:HE2	1:C:217:LEU:O	2.12	0.48
1:C:91:VAL:HG11	1:C:123:VAL:HG11	1.96	0.48
1:D:17:VAL:O	1:D:17:VAL:CG2	2.61	0.48
1:D:18:PRO:HB2	1:D:21:LYS:HB2	1.96	0.48
1:E:304:LYS:HE3	1:F:6:GLN:O	2.13	0.48
1:F:206:ALA:HA	1:G:187:TRP:CZ2	2.49	0.48
1:G:103:GLU:OE1	1:G:107:ASN:OD1	2.32	0.48
1:G:279:LEU:HD13	1:G:302:VAL:HG21	1.93	0.48
1:E:187:TRP:CZ2	1:H:206:ALA:HA	2.48	0.48
1:G:10:ASN:HA	1:H:301:ASP:OD2	2.13	0.48
1:H:29:ALA:CB	1:H:248:THR:HG21	2.35	0.48
1:A:302:VAL:HG13	1:B:11:LEU:HD11	1.96	0.48
1:D:214:HIS:CE1	1:D:216:GLU:HB2	2.49	0.48
1:G:127:SER:HB3	1:G:130:CYS:HB3	1.96	0.48
1:H:51:ASP:OD1	1:H:52:VAL:N	2.47	0.48
1:D:61:MET:O	1:D:65:GLN:HG3	2.13	0.48
1:G:110:GLN:O	1:G:114:ASN:N	2.43	0.48
1:B:33:ALA:HB2	1:B:248:THR:HB	1.95	0.48
1:B:318:SER:O	1:B:322:LEU:HG	2.14	0.48
1:F:103:GLU:O	1:F:104:SER:CB	2.62	0.48
1:H:158:ILE:N	1:H:158:ILE:HD12	2.29	0.48
1:D:276:LEU:C	1:D:276:LEU:HD13	2.34	0.48
1:A:117:LYS:HA	1:A:117:LYS:HZ3	1.79	0.47
1:G:316:LYS:HG3	1:G:316:LYS:O	2.12	0.47
1:C:109:VAL:O	1:C:113:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:MET:CE	1:E:60:GLU:HB3	2.45	0.47
1:F:283:LYS:HA	1:F:283:LYS:HE3	1.96	0.47
1:G:246:TYR:HD2	1:G:248:THR:HG23	1.79	0.47
1:H:179:VAL:HG12	1:H:180:HIS:N	2.28	0.47
1:B:48:ALA:HA	1:B:77:VAL:O	2.15	0.47
1:D:16:HIS:HE1	1:D:75:LYS:HD2	1.79	0.47
1:E:86:ALA:O	1:E:87:ASN:HB2	2.14	0.47
1:A:169:PHE:CE2	1:A:229:VAL:HG12	2.49	0.47
1:B:50:VAL:HG23	1:B:79:GLY:O	2.14	0.47
1:D:248:THR:O	1:D:251:ILE:HG22	2.14	0.47
1:B:121:PRO:HA	1:B:124:VAL:HG22	1.96	0.47
1:B:12:LEU:HG	1:B:14:GLU:CB	2.36	0.47
1:C:240:VAL:CG1	1:C:247:THR:HG22	2.45	0.47
1:E:139:VAL:HG13	1:E:140:ASP:N	2.29	0.47
1:E:166:SER:O	1:E:170:ARG:HG3	2.15	0.47
1:E:239:GLU:HA	1:E:242:LYS:HE3	1.96	0.47
1:F:246:TYR:CD2	1:F:248:THR:HG23	2.49	0.47
1:G:228:GLN:HE22	1:G:231:LYS:HD3	1.79	0.47
1:E:282:ILE:HD12	1:E:319:ALA:HB2	1.97	0.47
1:E:22:ILE:HD12	1:E:44:ALA:HB2	1.95	0.47
1:E:301:ASP:OD2	1:F:10:ASN:HA	2.14	0.47
1:F:110:GLN:OE1	1:F:329:LEU:HA	2.14	0.47
1:A:189:LEU:HD22	1:A:290:VAL:HA	1.97	0.47
1:H:240:VAL:HB	1:H:247:THR:HG22	1.97	0.47
1:B:126:TYR:C	1:B:128:PRO:HD3	2.35	0.47
1:C:189:LEU:HD22	1:C:290:VAL:HA	1.96	0.47
1:D:238:TYR:CE2	1:D:242:LYS:HE2	2.50	0.47
1:G:110:GLN:NE2	1:G:330:GLN:O	2.47	0.47
1:G:82:TYR:CG	1:G:122:ASN:HB3	2.49	0.47
1:H:126:TYR:C	1:H:128:PRO:HD3	2.35	0.47
1:H:155:ASN:O	1:H:298:GLY:HA3	2.14	0.47
1:D:91:VAL:HG11	1:D:123:VAL:HG11	1.97	0.47
1:E:81:ASP:OD1	1:E:81:ASP:C	2.53	0.47
1:F:147:TRP:HA	1:F:157:VAL:HG21	1.97	0.47
1:H:12:LEU:CD2	1:H:13:LYS:HE2	2.42	0.47
1:C:105:ARG:NH1	1:C:325:ILE:HD11	2.30	0.47
1:F:325:ILE:O	1:F:329:LEU:HD13	2.14	0.47
1:G:141:ILE:O	1:G:144:TYR:HB3	2.15	0.47
1:A:276:LEU:HD21	1:A:288:LEU:HD12	1.96	0.46
1:B:99:GLN:OE1	1:B:103:GLU:HB2	2.15	0.46
1:F:113:VAL:HG21	1:F:329:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:SER:HA	1:F:288:LEU:O	2.16	0.46
1:E:12:LEU:HB2	1:F:300:SER:HA	1.95	0.46
1:C:238:TYR:CE1	1:C:242:LYS:HD2	2.50	0.46
1:E:261:SER:HA	1:E:266:LEU:HD12	1.97	0.46
1:F:97:ALA:HB1	1:F:111:ARG:NH2	2.31	0.46
1:F:216:GLU:OE1	1:F:223:LYS:HE2	2.16	0.46
1:F:51:ASP:OD1	1:F:53:MET:HG3	2.15	0.46
1:H:49:LEU:O	1:H:78:SER:HA	2.16	0.46
1:B:105:ARG:C	1:B:107:ASN:H	2.15	0.46
1:B:141:ILE:HD11	1:B:325:ILE:HD12	1.98	0.46
1:H:50:VAL:HG21	1:H:82:TYR:CE2	2.50	0.46
1:H:82:TYR:OH	1:H:119:ILE:HG12	2.14	0.46
1:A:117:LYS:NZ	1:A:117:LYS:HA	2.30	0.46
1:A:145:VAL:HG12	1:A:149:ILE:HD12	1.97	0.46
1:E:98:ARG:CZ	1:E:111:ARG:NH2	2.79	0.46
1:E:40:MET:HE1	1:G:37:SER:HA	1.98	0.46
1:A:185:HIS:O	1:A:203:MET:HA	2.16	0.46
1:C:240:VAL:HG11	1:C:247:THR:HG22	1.97	0.46
1:D:86:ALA:HA	1:D:126:TYR:HB3	1.97	0.46
1:F:141:ILE:HG22	1:F:142:LEU:N	2.30	0.46
1:A:69:LEU:HD22	1:C:167:ALA:HA	1.96	0.46
1:D:101:GLU:N	1:D:102:GLY:HA3	2.30	0.46
1:D:272:ILE:O	1:D:289:SER:HA	2.15	0.46
1:E:275:MET:HE1	1:E:277:LYS:HB3	1.98	0.46
1:B:141:ILE:HD13	1:B:325:ILE:HG21	1.97	0.46
1:G:185:HIS:O	1:G:203:MET:HA	2.16	0.46
1:B:32:MET:HE2	1:B:60:GLU:OE1	2.16	0.46
1:D:145:VAL:HG22	1:D:331:PHE:CZ	2.50	0.46
1:D:110:GLN:HE22	1:D:330:GLN:H	1.64	0.46
1:H:18:PRO:HB2	1:H:21:LYS:HB2	1.98	0.46
1:E:300:SER:O	1:F:11:LEU:HB2	2.16	0.46
1:G:225:GLN:HB3	1:G:228:GLN:HG2	1.98	0.46
1:B:141:ILE:CD1	1:B:325:ILE:HG21	2.46	0.45
1:B:321:THR:O	1:B:325:ILE:HG13	2.16	0.45
1:F:46:GLU:OE2	1:F:75:LYS:HE3	2.16	0.45
1:A:211:LYS:O	1:A:211:LYS:HG3	2.15	0.45
1:B:97:ALA:HB2	1:B:115:ILE:HD11	1.98	0.45
1:D:321:THR:O	1:D:325:ILE:HG13	2.15	0.45
1:E:136:SER:O	1:E:139:VAL:HA	2.17	0.45
1:G:136:SER:HB2	1:G:142:LEU:CD1	2.46	0.45
1:G:191:GLU:HB2	1:G:318:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:THR:HB	1:A:299:ILE:HD13	1.97	0.45
1:C:105:ARG:CZ	1:C:325:ILE:CD1	2.95	0.45
1:D:196:SER:OG	1:D:230:HIS:HE1	2.00	0.45
1:E:282:ILE:HD12	1:E:319:ALA:HB3	1.98	0.45
1:E:57:LEU:HG	1:E:78:SER:HB2	1.97	0.45
1:F:228:GLN:NE2	1:F:231:LYS:HD3	2.32	0.45
1:B:171:TYR:HA	1:B:181:ALA:HB2	1.98	0.45
1:C:170:ARG:HA	1:C:173:MET:HE3	1.98	0.45
1:F:103:GLU:O	1:F:104:SER:OG	2.25	0.45
1:F:60:GLU:OE1	1:F:60:GLU:HA	2.16	0.45
1:H:273:SER:HA	1:H:288:LEU:O	2.15	0.45
1:A:282:ILE:HD13	1:A:288:LEU:HD12	1.97	0.45
1:A:50:VAL:HG11	1:A:82:TYR:CZ	2.52	0.45
1:B:12:LEU:CG	1:B:14:GLU:HB2	2.36	0.45
1:B:166:SER:O	1:B:170:ARG:HG3	2.16	0.45
1:B:16:HIS:CD2	1:B:16:HIS:N	2.82	0.45
1:C:232:GLN:O	1:C:236:SER:HB3	2.16	0.45
1:C:22:ILE:O	1:C:47:LEU:HA	2.17	0.45
1:F:141:ILE:O	1:F:144:TYR:HB3	2.17	0.45
1:G:136:SER:O	1:G:139:VAL:HA	2.16	0.45
1:G:110:GLN:HE22	1:G:330:GLN:CA	2.30	0.45
1:H:185:HIS:O	1:H:203:MET:HA	2.16	0.45
1:B:82:TYR:CG	1:B:122:ASN:HB3	2.52	0.45
1:D:98:ARG:HE	1:D:99:GLN:H	1.63	0.45
1:E:182:LEU:HD13	1:H:268:ARG:HD3	1.97	0.45
1:B:66:HIS:HB3	1:D:168:ARG:HG2	1.99	0.45
1:H:240:VAL:HB	1:H:247:THR:CG2	2.47	0.45
1:A:261:SER:HA	1:A:266:LEU:HD12	1.99	0.45
1:E:164:LEU:HD12	1:E:164:LEU:O	2.17	0.45
1:E:162:CYS:HB2	1:E:289:SER:CB	2.47	0.45
1:H:276:LEU:CD2	1:H:282:ILE:HD12	2.47	0.45
1:D:145:VAL:HG13	1:D:331:PHE:CE2	2.43	0.45
1:D:60:GLU:HA	1:D:60:GLU:OE1	2.17	0.45
1:H:56:LYS:O	1:H:60:GLU:HG2	2.17	0.45
1:C:145:VAL:HG12	1:C:149:ILE:HD12	1.97	0.44
1:B:49:LEU:O	1:B:78:SER:HA	2.16	0.44
1:C:284:GLU:OE1	1:C:284:GLU:HA	2.16	0.44
1:H:307:LEU:HD22	1:H:311:GLU:HB3	1.99	0.44
1:A:117:LYS:HE2	1:A:149:ILE:HD13	1.98	0.44
1:A:31:GLY:HA2	1:A:94:THR:HG21	2.00	0.44
1:D:22:ILE:CG1	1:D:44:ALA:HB2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:TYR:C	1:G:128:PRO:HD3	2.37	0.44
1:G:203:MET:HE2	1:G:217:LEU:HD21	1.99	0.44
1:H:97:ALA:N	1:H:112:ASN:HD21	2.11	0.44
1:C:274:THR:HB	1:C:299:ILE:HD13	1.99	0.44
1:F:117:LYS:HA	1:F:149:ILE:HD13	1.99	0.44
1:E:155:ASN:ND2	1:F:12:LEU:HD11	2.33	0.44
1:E:206:ALA:HA	1:H:187:TRP:CE2	2.52	0.44
1:B:144:TYR:O	1:B:147:TRP:HB3	2.18	0.44
1:D:105:ARG:HB3	1:D:105:ARG:CZ	2.47	0.44
1:D:48:ALA:HA	1:D:77:VAL:O	2.18	0.44
1:E:251:ILE:HG23	1:E:252:GLY:N	2.33	0.44
1:B:17:VAL:O	1:B:17:VAL:HG13	2.17	0.44
1:E:210:LEU:HD21	1:G:7:LEU:HD22	1.97	0.44
1:G:276:LEU:HD12	1:G:276:LEU:N	2.26	0.44
1:E:18:PRO:HB2	1:E:21:LYS:HB2	1.99	0.44
1:F:96:GLY:HA2	1:F:112:ASN:HD22	1.82	0.44
1:H:316:LYS:HE3	1:H:320:ASP:OD1	2.17	0.44
1:H:34:CYS:O	1:H:38:ILE:HG13	2.17	0.44
1:A:164:LEU:HD12	1:A:167:ALA:HB3	2.00	0.44
1:A:194:ASP:HA	1:A:234:VAL:CG1	2.46	0.44
1:C:211:LYS:HD3	1:C:217:LEU:HB3	1.99	0.44
1:C:230:HIS:O	1:C:233:VAL:HB	2.18	0.44
1:D:189:LEU:HD12	1:D:199:VAL:HG21	1.99	0.44
1:D:277:LYS:HD3	1:D:284:GLU:C	2.38	0.44
1:C:102:GLY:O	1:C:103:GLU:C	2.57	0.43
1:D:204:ASN:HD22	1:D:207:GLY:N	2.13	0.43
1:E:98:ARG:NH2	1:E:111:ARG:NH2	2.66	0.43
1:F:141:ILE:CD1	1:F:322:LEU:HD22	2.47	0.43
1:G:16:HIS:CE1	1:G:75:LYS:HZ2	2.36	0.43
1:H:129:HIS:C	1:H:156:ARG:NH1	2.72	0.43
1:A:317:LYS:HB3	3:A:525:HOH:O	2.18	0.43
1:A:300:SER:HB2	1:B:12:LEU:HB3	1.99	0.43
1:C:232:GLN:NE2	3:C:511:HOH:O	2.48	0.43
1:C:105:ARG:CZ	1:C:325:ILE:HD13	2.48	0.43
1:D:101:GLU:H	1:D:102:GLY:HA3	1.83	0.43
1:D:144:TYR:O	1:D:147:TRP:HB3	2.18	0.43
1:F:291:PRO:HB2	1:F:303:VAL:HB	1.99	0.43
1:F:22:ILE:HG13	1:F:44:ALA:HB2	2.01	0.43
1:H:107:ASN:O	1:H:111:ARG:HG3	2.18	0.43
1:A:226:TRP:O	1:A:229:VAL:HB	2.18	0.43
1:B:97:ALA:HB1	1:B:111:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:TRP:HE3	1:D:203:MET:SD	2.41	0.43
1:E:74:PRO:O	1:E:75:LYS:HE3	2.18	0.43
1:G:136:SER:HB2	1:G:142:LEU:HD12	2.00	0.43
1:D:219:THR:HG23	1:D:222:ASP:N	2.33	0.43
1:E:124:VAL:HG22	1:E:152:PHE:CZ	2.53	0.43
1:F:276:LEU:O	1:F:276:LEU:HD13	2.18	0.43
1:H:200:TRP:CE3	1:H:203:MET:SD	3.12	0.43
1:A:246:TYR:CD2	1:A:248:THR:HG23	2.53	0.43
1:A:98:ARG:HG3	1:A:111:ARG:HH12	1.83	0.43
1:C:276:LEU:HD11	1:C:282:ILE:HG21	2.00	0.43
1:F:158:ILE:HD12	1:F:158:ILE:N	2.32	0.43
1:H:279:LEU:HD13	1:H:279:LEU:HA	1.73	0.43
1:B:141:ILE:O	1:B:145:VAL:HG23	2.18	0.43
1:D:179:VAL:CG1	1:D:180:HIS:N	2.82	0.43
1:F:242:LYS:HE3	3:F:521:HOH:O	2.19	0.43
1:C:169:PHE:HB2	1:C:188:ILE:HD11	2.01	0.43
1:F:251:ILE:O	1:F:255:VAL:HG23	2.19	0.43
1:E:58:LYS:HB3	1:G:243:LEU:HD13	2.01	0.43
1:B:75:LYS:HE3	1:B:75:LYS:HB2	1.80	0.43
1:G:173:MET:HE2	1:G:173:MET:HB2	1.67	0.43
1:H:241:ILE:HG13	1:H:247:THR:HG23	2.01	0.43
1:G:132:LEU:HD12	1:G:157:VAL:HG22	2.01	0.43
1:H:279:LEU:HD12	1:H:280:TYR:H	1.84	0.43
1:E:117:LYS:HA	1:E:149:ILE:HD13	2.01	0.43
1:G:228:GLN:NE2	1:G:231:LYS:HD3	2.33	0.43
1:H:164:LEU:O	1:H:168:ARG:HG3	2.19	0.43
1:H:105:ARG:HG2	1:H:325:ILE:HD13	2.01	0.43
1:C:155:ASN:O	1:C:298:GLY:HA3	2.18	0.42
1:E:189:LEU:HD22	1:E:291:PRO:HD3	2.01	0.42
1:E:33:ALA:O	1:E:36:ILE:HG22	2.19	0.42
1:G:21:LYS:HB3	1:G:88:SER:HA	2.00	0.42
1:D:223:LYS:CD	1:D:223:LYS:H	2.28	0.42
1:D:260:GLU:O	1:D:264:LYS:HB2	2.19	0.42
1:E:205:VAL:O	1:E:206:ALA:HB3	2.19	0.42
1:D:105:ARG:NH1	1:D:105:ARG:HB2	2.34	0.42
1:E:153:PRO:HG2	1:E:156:ARG:HG3	2.00	0.42
1:F:158:ILE:HG23	1:F:272:ILE:HD12	2.00	0.42
1:F:206:ALA:HA	1:G:187:TRP:CE2	2.54	0.42
1:G:28:GLY:O	1:G:29:ALA:C	2.57	0.42
1:B:189:LEU:HD22	1:B:290:VAL:HA	1.99	0.42
1:C:139:VAL:HG13	1:C:140:ASP:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:TRP:CE3	1:D:203:MET:SD	3.12	0.42
1:A:187:TRP:CE2	1:D:206:ALA:HA	2.54	0.42
1:E:120:ILE:HB	1:E:121:PRO:HD3	2.02	0.42
1:G:13:LYS:HE3	1:G:14:GLU:OE1	2.20	0.42
1:E:40:MET:CE	1:G:40:MET:HB2	2.49	0.42
1:H:204:ASN:HD22	1:H:207:GLY:H	1.65	0.42
1:D:204:ASN:HA	1:D:210:LEU:HD13	2.01	0.42
1:D:29:ALA:CB	1:D:248:THR:CG2	2.95	0.42
1:H:92:ILE:HG22	1:H:94:THR:HG23	2.00	0.42
1:A:187:TRP:CZ2	1:D:206:ALA:HA	2.55	0.42
1:C:307:LEU:HB3	1:C:311:GLU:HB2	2.00	0.42
1:E:258:LEU:O	1:E:262:ILE:HG13	2.19	0.42
1:H:58:LYS:O	1:H:62:MET:HG3	2.18	0.42
1:A:206:ALA:HA	1:D:187:TRP:CE2	2.55	0.42
1:B:248:THR:O	1:B:251:ILE:HG23	2.19	0.42
1:D:145:VAL:HG22	1:D:331:PHE:CE2	2.55	0.42
1:D:180:HIS:ND1	1:D:181:ALA:N	2.67	0.42
1:F:200:TRP:CE3	1:F:203:MET:SD	3.12	0.42
1:E:60:GLU:OE2	1:G:244:LYS:HE3	2.20	0.42
1:A:22:ILE:O	1:A:47:LEU:HA	2.19	0.42
1:B:99:GLN:HG3	1:B:100:GLN:H	1.85	0.42
1:E:214:HIS:NE2	1:E:222:ASP:OD1	2.53	0.42
1:E:293:VAL:O	1:E:299:ILE:HA	2.19	0.42
1:H:9:HIS:HD2	1:H:11:LEU:HG	1.84	0.42
1:A:179:VAL:HG12	1:D:293:VAL:HG22	2.02	0.42
1:C:148:LYS:HD3	1:C:331:PHE:CZ	2.55	0.42
1:C:90:LEU:HD21	1:C:92:ILE:HD11	2.02	0.42
1:F:96:GLY:CA	1:F:112:ASN:ND2	2.83	0.42
1:A:141:ILE:O	1:A:145:VAL:HG23	2.20	0.42
1:A:14:GLU:OE2	1:B:297:ASN:OD1	2.38	0.42
1:A:328:GLU:O	1:A:329:LEU:C	2.59	0.42
1:B:10:ASN:OD1	1:B:13:LYS:HG2	2.20	0.42
1:C:164:LEU:HD11	1:C:250:ALA:HB1	2.02	0.42
1:C:164:LEU:HG	1:C:168:ARG:NH2	2.35	0.42
1:C:165:ASP:O	1:C:168:ARG:HB2	2.20	0.42
1:D:238:TYR:CZ	1:D:242:LYS:HE2	2.55	0.42
1:D:266:LEU:O	1:D:267:ARG:HB2	2.19	0.42
1:F:60:GLU:OE1	1:H:244:LYS:NZ	2.44	0.42
1:E:264:LYS:O	1:F:74:PRO:HG3	2.19	0.42
1:A:83:SER:HA	1:A:126:TYR:CE2	2.55	0.41
1:B:308:THR:O	1:B:312:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:VAL:HB	1:C:247:THR:CG2	2.50	0.41
1:F:169:PHE:CG	1:F:188:ILE:HD11	2.55	0.41
1:B:276:LEU:HD21	1:B:288:LEU:HD12	2.02	0.41
1:E:282:ILE:HG23	1:E:319:ALA:CB	2.50	0.41
1:F:120:ILE:O	1:F:124:VAL:HG23	2.21	0.41
1:F:27:VAL:HG11	1:F:57:LEU:HD13	2.01	0.41
1:G:14:GLU:O	1:G:14:GLU:CD	2.58	0.41
1:B:244:LYS:HG3	1:B:246:TYR:O	2.21	0.41
1:C:158:ILE:HD12	1:C:158:ILE:N	2.35	0.41
1:C:19:GLN:HG2	1:D:296:GLN:OE1	2.21	0.41
1:C:98:ARG:CG	1:C:98:ARG:HH21	2.33	0.41
1:D:144:TYR:CD2	1:D:326:GLN:HG2	2.55	0.41
1:E:104:SER:C	1:E:106:LEU:N	2.73	0.41
1:F:115:ILE:HG22	1:F:119:ILE:HD12	2.02	0.41
1:G:158:ILE:CG2	1:G:272:ILE:HD12	2.49	0.41
1:H:148:LYS:HD2	1:H:148:LYS:HA	1.62	0.41
1:H:276:LEU:HD21	1:H:282:ILE:HD12	2.02	0.41
1:B:86:ALA:HA	1:B:126:TYR:HB3	2.02	0.41
1:C:211:LYS:HD2	1:C:217:LEU:HB3	2.03	0.41
1:E:107:ASN:O	1:E:111:ARG:HG3	2.20	0.41
1:F:47:LEU:O	1:F:76:ILE:HA	2.20	0.41
1:G:179:VAL:CG2	1:G:184:CYS:SG	3.09	0.41
1:G:282:ILE:N	1:G:282:ILE:HD12	2.34	0.41
1:B:107:ASN:HA	1:B:107:ASN:HD22	1.62	0.41
1:B:136:SER:O	1:B:139:VAL:HA	2.20	0.41
1:B:16:HIS:CD2	1:B:16:HIS:H	2.38	0.41
1:B:211:LYS:O	1:B:211:LYS:HG3	2.20	0.41
1:D:251:ILE:O	1:D:255:VAL:HG23	2.20	0.41
1:F:100:GLN:O	1:F:101:GLU:C	2.58	0.41
1:F:309:SER:O	1:F:312:GLU:HB2	2.21	0.41
1:G:106:LEU:HD11	1:G:328:GLU:HB3	2.02	0.41
1:G:56:LYS:O	1:G:60:GLU:HG2	2.21	0.41
1:A:204:ASN:HD22	1:A:207:GLY:H	1.68	0.41
1:D:291:PRO:HB2	1:D:303:VAL:HB	2.03	0.41
1:E:12:LEU:HD23	1:E:12:LEU:HA	1.88	0.41
1:E:180:HIS:CE1	1:E:182:LEU:HG	2.56	0.41
1:F:23:THR:HG23	1:F:48:ALA:O	2.19	0.41
1:G:280:TYR:O	1:G:282:ILE:HD12	2.20	0.41
1:A:110:GLN:HA	1:A:113:VAL:HB	2.02	0.41
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.79	0.41
1:E:111:ARG:O	1:E:114:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:VAL:O	1:G:113:VAL:N	2.43	0.41
1:G:117:LYS:HE2	1:G:117:LYS:HB3	1.85	0.41
1:G:322:LEU:HD12	1:G:322:LEU:HA	1.78	0.41
1:G:327:LYS:HE3	1:G:327:LYS:HB2	1.63	0.41
1:H:12:LEU:HD23	1:H:12:LEU:HA	1.71	0.41
1:H:180:HIS:CE1	1:H:182:LEU:HG	2.56	0.41
1:B:142:LEU:HD23	1:B:142:LEU:HA	1.77	0.41
1:B:34:CYS:O	1:B:38:ILE:HG13	2.21	0.41
1:C:136:SER:O	1:C:139:VAL:HA	2.21	0.41
1:C:300:SER:OG	1:C:301:ASP:OD1	2.34	0.41
1:E:163:ASN:HB3	3:E:514:HOH:O	2.20	0.41
1:G:34:CYS:O	1:G:38:ILE:HG13	2.21	0.41
1:G:50:VAL:HG11	1:G:82:TYR:CZ	2.55	0.41
1:H:218:GLY:O	1:H:227:LYS:HB2	2.21	0.41
1:E:80:LYS:NZ	1:E:80:LYS:HB3	2.35	0.41
1:G:82:TYR:CZ	1:G:119:ILE:HG23	2.56	0.41
1:H:282:ILE:CD1	1:H:288:LEU:HD12	2.51	0.41
1:B:105:ARG:HD3	1:B:325:ILE:HD13	2.03	0.41
1:B:86:ALA:O	1:B:87:ASN:HB2	2.21	0.41
1:C:99:GLN:HA	1:C:108:LEU:HD13	2.03	0.41
1:C:216:GLU:O	1:C:222:ASP:HB2	2.21	0.41
1:F:187:TRP:CZ2	1:G:206:ALA:HA	2.55	0.41
1:F:27:VAL:HG11	1:F:57:LEU:CD1	2.51	0.41
1:G:155:ASN:O	1:G:298:GLY:HA3	2.21	0.41
1:H:39:LEU:HB3	1:H:71:LEU:HD22	2.02	0.41
1:H:89:LYS:HA	1:H:89:LYS:HD3	1.81	0.41
1:C:142:LEU:HA	1:C:142:LEU:HD23	1.86	0.41
1:D:216:GLU:O	1:D:217:LEU:C	2.60	0.41
1:A:180:HIS:HB2	1:D:266:LEU:O	2.21	0.41
1:G:279:LEU:HD11	1:H:9:HIS:CD2	2.56	0.41
1:H:238:TYR:CD2	1:H:239:GLU:N	2.89	0.41
1:E:327:LYS:NZ	1:E:327:LYS:CB	2.84	0.40
1:F:276:LEU:CD1	1:F:276:LEU:C	2.89	0.40
1:H:315:LEU:HA	1:H:315:LEU:HD12	1.91	0.40
1:H:36:ILE:O	1:H:40:MET:HG3	2.21	0.40
1:F:45:ASP:O	1:F:74:PRO:HD2	2.20	0.40
1:G:193:GLY:O	1:G:234:VAL:HG22	2.22	0.40
1:H:14:GLU:C	1:H:15:GLU:HG2	2.41	0.40
1:H:71:LEU:C	1:H:72:ARG:HD2	2.41	0.40
1:E:204:ASN:HA	1:E:210:LEU:HG	2.03	0.40
1:F:166:SER:O	1:F:170:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:253:LEU:HD12	1:H:67:GLY:HA3	2.02	0.40
1:F:158:ILE:HG21	1:F:272:ILE:HD12	2.03	0.40
1:H:110:GLN:NE2	1:H:330:GLN:H	2.16	0.40
1:B:145:VAL:HG13	1:B:331:PHE:CE2	2.52	0.40
1:B:155:ASN:O	1:B:298:GLY:HA3	2.21	0.40
1:B:14:GLU:CG	1:B:15:GLU:H	2.19	0.40
1:B:211:LYS:HE3	1:B:217:LEU:HB3	2.02	0.40
1:F:116:PHE:HE2	1:F:142:LEU:O	2.04	0.40
1:G:110:GLN:HE22	1:G:330:GLN:CB	2.35	0.40
1:G:22:ILE:HD12	1:G:44:ALA:HB2	2.03	0.40
1:G:75:LYS:HE3	1:G:75:LYS:HB2	1.52	0.40
1:H:114:ASN:HA	1:H:117:LYS:HD3	2.03	0.40
1:H:48:ALA:HA	1:H:77:VAL:O	2.22	0.40
1:A:292:CYS:SG	1:A:299:ILE:HD13	2.62	0.40
1:C:113:VAL:HG21	1:C:329:LEU:HD13	2.04	0.40
1:C:200:TRP:HH2	1:C:226:TRP:O	2.05	0.40
1:C:22:ILE:HG13	1:C:44:ALA:HB2	2.03	0.40
1:D:197:VAL:HG21	1:D:315:LEU:HD21	2.02	0.40
1:D:98:ARG:NE	1:D:98:ARG:HA	2.37	0.40
1:F:214:HIS:CE1	1:F:216:GLU:HB2	2.56	0.40
1:F:21:LYS:HD2	1:F:46:GLU:CD	2.42	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/331 (96%)	305 (96%)	10 (3%)	4 (1%)	12	21
1	B	329/331 (99%)	309 (94%)	14 (4%)	6 (2%)	8	14
1	C	329/331 (99%)	310 (94%)	18 (6%)	1 (0%)	41	61
1	D	329/331 (99%)	316 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	329/331 (99%)	312 (95%)	16 (5%)	1 (0%)	41	61
1	F	325/331 (98%)	302 (93%)	18 (6%)	5 (2%)	10	18
1	G	322/331 (97%)	308 (96%)	13 (4%)	1 (0%)	41	61
1	H	322/331 (97%)	305 (95%)	14 (4%)	3 (1%)	17	31
All	All	2604/2648 (98%)	2467 (95%)	116 (4%)	21 (1%)	19	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	329	LEU
1	B	101	GLU
1	B	104	SER
1	B	105	ARG
1	B	106	LEU
1	F	104	SER
1	F	105	ARG
1	G	14	GLU
1	H	104	SER
1	B	16	HIS
1	C	104	SER
1	F	101	GLU
1	F	136	SER
1	A	328	GLU
1	F	53	MET
1	H	16	HIS
1	B	100	GLN
1	E	248	THR
1	A	248	THR
1	H	13	LYS

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	277/284 (98%)	266 (96%)	11 (4%)	31	56
1	B	284/284 (100%)	266 (94%)	18 (6%)	18	34
1	C	284/284 (100%)	276 (97%)	8 (3%)	43	70
1	D	284/284 (100%)	277 (98%)	7 (2%)	47	73
1	E	284/284 (100%)	273 (96%)	11 (4%)	32	57
1	F	282/284 (99%)	271 (96%)	11 (4%)	32	57
1	G	280/284 (99%)	266 (95%)	14 (5%)	24	46
1	H	280/284 (99%)	269 (96%)	11 (4%)	32	57
All	All	2255/2272 (99%)	2164 (96%)	91 (4%)	31	56

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ARG
1	A	98	ARG
1	A	117	LYS
1	A	133	LEU
1	A	136	SER
1	A	148	LYS
1	A	194	ASP
1	A	211	LYS
1	A	276	LEU
1	A	315	LEU
1	A	330	GLN
1	B	80	LYS
1	B	89	LYS
1	B	98	ARG
1	B	100	GLN
1	B	103	GLU
1	B	106	LEU
1	B	108	LEU
1	B	117	LYS
1	B	194	ASP
1	B	211	LYS
1	B	223	LYS
1	B	236	SER
1	B	273	SER
1	B	276	LEU
1	B	277	LYS
1	B	315	LEU

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Mol	Chain	Res	Type
1	B	329	LEU
1	B	330	GLN
1	C	14	GLU
1	C	15	GLU
1	C	68	SER
1	C	98	ARG
1	C	194	ASP
1	C	220	ASP
1	C	238	TYR
1	C	276	LEU
1	D	14	GLU
1	D	17	VAL
1	D	223	LYS
1	D	276	LEU
1	D	285	ASP
1	D	301	ASP
1	D	310	GLU
1	E	12	LEU
1	E	14	GLU
1	E	50	VAL
1	E	75	LYS
1	E	81	ASP
1	E	98	ARG
1	E	105	ARG
1	E	194	ASP
1	E	276	LEU
1	E	283	LYS
1	E	317	LYS
1	F	13	LYS
1	F	19	GLN
1	F	98	ARG
1	F	110	GLN
1	F	141	ILE
1	F	173	MET
1	F	220	ASP
1	F	223	LYS
1	F	276	LEU
1	F	283	LYS
1	F	316	LYS
1	G	12	LEU
1	G	13	LYS
1	G	14	GLU

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Mol	Chain	Res	Type
1	G	17	VAL
1	G	81	ASP
1	G	105	ARG
1	G	108	LEU
1	G	173	MET
1	G	219	THR
1	G	276	LEU
1	G	314	HIS
1	G	316	LYS
1	G	322	LEU
1	G	330	GLN
1	H	12	LEU
1	H	13	LYS
1	H	75	LYS
1	H	131	LYS
1	H	148	LYS
1	H	223	LYS
1	H	238	TYR
1	H	276	LEU
1	H	279	LEU
1	H	310	GLU
1	H	318	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	9	HIS
1	A	112	ASN
1	A	204	ASN
1	A	230	HIS
1	A	326	GLN
1	A	330	GLN
1	B	9	HIS
1	B	16	HIS
1	B	107	ASN
1	B	112	ASN
1	B	204	ASN
1	B	214	HIS
1	B	230	HIS
1	C	6	GLN
1	C	107	ASN

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Mol	Chain	Res	Type
1	C	110	GLN
1	C	112	ASN
1	C	122	ASN
1	C	192	HIS
1	C	204	ASN
1	C	228	GLN
1	C	230	HIS
1	D	16	HIS
1	D	19	GLN
1	D	107	ASN
1	D	110	GLN
1	D	112	ASN
1	D	122	ASN
1	D	204	ASN
1	D	228	GLN
1	D	230	HIS
1	D	297	ASN
1	D	330	GLN
1	E	9	HIS
1	E	16	HIS
1	E	20	ASN
1	E	87	ASN
1	E	100	GLN
1	E	112	ASN
1	E	163	ASN
1	E	204	ASN
1	F	20	ASN
1	F	87	ASN
1	F	100	GLN
1	F	112	ASN
1	F	204	ASN
1	F	214	HIS
1	F	225	GLN
1	F	228	GLN
1	F	230	HIS
1	G	9	HIS
1	G	20	ASN
1	G	112	ASN
1	G	204	ASN
1	G	225	GLN
1	G	228	GLN
1	G	230	HIS

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Mol	Chain	Res	Type
1	H	6	GLN
1	H	9	HIS
1	H	20	ASN
1	H	110	GLN
1	H	112	ASN
1	H	114	ASN
1	H	185	HIS
1	H	204	ASN
1	H	230	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	1E7	E	401	-	22,24,24	3.82	16 (72%)	28,32,32	1.33	4 (14%)
2	1E7	C	401	-	22,24,24	3.61	17 (77%)	28,32,32	1.35	3 (10%)
2	1E7	A	401	-	22,24,24	3.83	18 (81%)	28,32,32	1.27	3 (10%)
2	1E7	D	401	-	22,24,24	3.44	16 (72%)	28,32,32	1.27	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1E7	B	401	-	22,24,24	3.39	15 (68%)	28,32,32	1.16	2 (7%)
2	1E7	H	401	-	22,24,24	3.44	17 (77%)	28,32,32	1.20	3 (10%)
2	1E7	F	401	-	22,24,24	3.61	17 (77%)	28,32,32	1.30	4 (14%)
2	1E7	G	401	-	22,24,24	3.34	16 (72%)	28,32,32	1.28	3 (10%)

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	1E7	E	401	-	-	0/11/15/15	0/2/2/2
2	1E7	C	401	-	-	0/11/15/15	0/2/2/2
2	1E7	A	401	-	-	0/11/15/15	0/2/2/2
2	1E7	D	401	-	-	0/11/15/15	0/2/2/2
2	1E7	B	401	-	-	2/11/15/15	0/2/2/2
2	1E7	H	401	-	-	0/11/15/15	0/2/2/2
2	1E7	F	401	-	-	2/11/15/15	0/2/2/2
2	1E7	G	401	-	-	0/11/15/15	0/2/2/2

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	1E7	C13-C19	8.55	1.55	1.47
2	A	401	1E7	C13-C19	7.51	1.54	1.47
2	C	401	1E7	C13-C19	6.84	1.54	1.47
2	D	401	1E7	C13-C19	6.69	1.53	1.47
2	F	401	1E7	C13-C19	6.41	1.53	1.47
2	A	401	1E7	C23-C24	6.11	1.48	1.38
2	H	401	1E7	C13-C19	6.03	1.53	1.47
2	B	401	1E7	C23-C24	5.98	1.48	1.38
2	H	401	1E7	C23-C24	5.89	1.48	1.38
2	G	401	1E7	C13-C19	5.80	1.53	1.47
2	B	401	1E7	C13-C19	5.78	1.53	1.47
2	E	401	1E7	O31-C27	5.77	1.46	1.37
2	G	401	1E7	C23-C24	5.59	1.47	1.38
2	C	401	1E7	O31-C27	5.49	1.45	1.37
2	C	401	1E7	C23-C24	5.43	1.47	1.38
2	D	401	1E7	C23-C24	5.42	1.47	1.38
2	F	401	1E7	C23-C24	5.38	1.47	1.38
2	E	401	1E7	C23-C24	5.37	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	1E7	C23-C3	5.36	1.47	1.39
2	F	401	1E7	O31-C27	5.27	1.45	1.37
2	C	401	1E7	C23-C3	5.24	1.47	1.39
2	A	401	1E7	C23-C3	5.12	1.47	1.39
2	H	401	1E7	C23-C3	5.10	1.47	1.39
2	B	401	1E7	C23-C3	5.00	1.47	1.39
2	B	401	1E7	O31-C27	4.98	1.45	1.37
2	H	401	1E7	O31-C27	4.95	1.45	1.37
2	G	401	1E7	C23-C3	4.95	1.47	1.39
2	A	401	1E7	C12-C11	4.88	1.47	1.38
2	A	401	1E7	C3-C27	4.77	1.50	1.40
2	C	401	1E7	C12-C11	4.72	1.47	1.38
2	F	401	1E7	C3-C27	4.68	1.50	1.40
2	A	401	1E7	O31-C27	4.65	1.44	1.37
2	E	401	1E7	C10-S7	4.61	1.84	1.76
2	D	401	1E7	C23-C3	4.60	1.46	1.39
2	D	401	1E7	O31-C27	4.53	1.44	1.37
2	E	401	1E7	C23-C3	4.44	1.46	1.39
2	E	401	1E7	C12-C11	4.43	1.46	1.38
2	F	401	1E7	C12-C11	4.42	1.46	1.38
2	C	401	1E7	C26-C27	4.33	1.48	1.39
2	G	401	1E7	C26-C27	4.32	1.48	1.39
2	E	401	1E7	C26-C27	4.26	1.48	1.39
2	E	401	1E7	C3-C27	4.26	1.49	1.40
2	A	401	1E7	C26-C27	4.24	1.48	1.39
2	G	401	1E7	C12-C11	4.24	1.46	1.38
2	B	401	1E7	C12-C11	4.24	1.46	1.38
2	A	401	1E7	C10-S7	4.22	1.83	1.76
2	E	401	1E7	C14-N15	4.21	1.43	1.34
2	G	401	1E7	O31-C27	4.11	1.43	1.37
2	A	401	1E7	C14-N15	4.08	1.43	1.34
2	C	401	1E7	C10-S7	4.03	1.83	1.76
2	H	401	1E7	C26-C27	4.02	1.48	1.39
2	D	401	1E7	C12-C11	4.01	1.46	1.38
2	D	401	1E7	C14-N15	4.00	1.42	1.34
2	D	401	1E7	C26-C27	4.00	1.47	1.39
2	H	401	1E7	C12-C11	3.98	1.46	1.38
2	B	401	1E7	C3-C27	3.98	1.48	1.40
2	H	401	1E7	C3-C27	3.89	1.48	1.40
2	F	401	1E7	C26-C27	3.88	1.47	1.39
2	C	401	1E7	C3-C27	3.85	1.48	1.40
2	B	401	1E7	C26-C27	3.83	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	1E7	C3-C27	3.80	1.48	1.40
2	D	401	1E7	C3-C27	3.78	1.48	1.40
2	C	401	1E7	C14-N15	3.75	1.42	1.34
2	D	401	1E7	C10-S7	3.75	1.82	1.76
2	G	401	1E7	C6-C1	3.70	1.55	1.51
2	D	401	1E7	C26-C25	3.65	1.45	1.38
2	F	401	1E7	C10-S7	3.64	1.82	1.76
2	F	401	1E7	C26-C25	3.63	1.45	1.38
2	F	401	1E7	C14-N15	3.58	1.42	1.34
2	H	401	1E7	C14-N15	3.58	1.42	1.34
2	B	401	1E7	C14-N15	3.57	1.41	1.34
2	A	401	1E7	C6-C1	3.53	1.55	1.51
2	H	401	1E7	C6-C1	3.52	1.55	1.51
2	F	401	1E7	C6-C1	3.50	1.55	1.51
2	D	401	1E7	C6-C1	3.47	1.55	1.51
2	A	401	1E7	C3-N2	3.46	1.48	1.41
2	B	401	1E7	C10-S7	3.44	1.82	1.76
2	G	401	1E7	C14-N15	3.43	1.41	1.34
2	B	401	1E7	C26-C25	3.36	1.44	1.38
2	C	401	1E7	C26-C25	3.36	1.44	1.38
2	C	401	1E7	C6-C1	3.28	1.55	1.51
2	E	401	1E7	C6-C1	3.25	1.55	1.51
2	E	401	1E7	C14-C13	3.25	1.45	1.39
2	G	401	1E7	C26-C25	3.18	1.44	1.38
2	E	401	1E7	C26-C25	3.17	1.44	1.38
2	H	401	1E7	O4-C1	3.06	1.29	1.23
2	E	401	1E7	O4-C1	3.04	1.29	1.23
2	A	401	1E7	C12-C13	3.04	1.45	1.39
2	D	401	1E7	C14-C13	3.02	1.44	1.39
2	F	401	1E7	C14-C13	3.00	1.44	1.39
2	H	401	1E7	C14-C13	2.97	1.44	1.39
2	H	401	1E7	C3-N2	2.95	1.47	1.41
2	B	401	1E7	C12-C13	2.91	1.45	1.39
2	F	401	1E7	C25-C24	2.91	1.43	1.38
2	F	401	1E7	O4-C1	2.88	1.29	1.23
2	G	401	1E7	C14-C13	2.88	1.44	1.39
2	H	401	1E7	C10-S7	2.87	1.81	1.76
2	A	401	1E7	C26-C25	2.87	1.44	1.38
2	A	401	1E7	C14-C13	2.86	1.44	1.39
2	A	401	1E7	O4-C1	2.85	1.29	1.23
2	D	401	1E7	O4-C1	2.84	1.29	1.23
2	H	401	1E7	C26-C25	2.83	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	1E7	C25-C24	2.83	1.43	1.38
2	B	401	1E7	C25-C24	2.83	1.43	1.38
2	B	401	1E7	C6-C1	2.82	1.54	1.51
2	G	401	1E7	C10-S7	2.82	1.81	1.76
2	F	401	1E7	C3-N2	2.80	1.47	1.41
2	F	401	1E7	C12-C13	2.79	1.45	1.39
2	C	401	1E7	O4-C1	2.78	1.28	1.23
2	C	401	1E7	C12-C13	2.67	1.45	1.39
2	E	401	1E7	C3-N2	2.61	1.46	1.41
2	C	401	1E7	C3-N2	2.61	1.46	1.41
2	G	401	1E7	O4-C1	2.57	1.28	1.23
2	B	401	1E7	O4-C1	2.54	1.28	1.23
2	G	401	1E7	C25-C24	2.54	1.42	1.38
2	D	401	1E7	C12-C13	2.53	1.44	1.39
2	C	401	1E7	C14-C13	2.53	1.43	1.39
2	H	401	1E7	C12-C13	2.52	1.44	1.39
2	B	401	1E7	C14-C13	2.52	1.43	1.39
2	G	401	1E7	C12-C13	2.51	1.44	1.39
2	H	401	1E7	C25-C24	2.44	1.42	1.38
2	E	401	1E7	C12-C13	2.38	1.44	1.39
2	G	401	1E7	C3-N2	2.32	1.46	1.41
2	E	401	1E7	C25-C24	2.32	1.42	1.38
2	A	401	1E7	C1-N2	2.27	1.40	1.35
2	A	401	1E7	C11-C10	2.26	1.44	1.39
2	D	401	1E7	C25-C24	2.13	1.42	1.38
2	D	401	1E7	C3-N2	2.11	1.45	1.41
2	H	401	1E7	C1-N2	2.11	1.40	1.35
2	C	401	1E7	C1-N2	2.10	1.40	1.35
2	F	401	1E7	C11-C10	2.04	1.44	1.39
2	C	401	1E7	C25-C24	2.04	1.41	1.38

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	1E7	C6-C1-N2	3.18	118.77	114.41
2	A	401	1E7	C6-C1-N2	2.96	118.47	114.41
2	C	401	1E7	C6-C1-N2	2.95	118.45	114.41
2	F	401	1E7	C6-C1-N2	2.84	118.31	114.41
2	C	401	1E7	C14-N15-C10	2.84	120.25	117.06
2	A	401	1E7	C14-N15-C10	2.70	120.10	117.06
2	E	401	1E7	C3-C23-C24	2.65	123.20	118.53
2	E	401	1E7	C6-C1-N2	2.65	118.04	114.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	1E7	C3-C23-C24	2.63	123.17	118.53
2	D	401	1E7	C6-C1-N2	2.63	118.01	114.41
2	G	401	1E7	C14-N15-C10	2.62	120.01	117.06
2	C	401	1E7	C3-C23-C24	2.56	123.04	118.53
2	F	401	1E7	O31-C27-C3	2.55	117.93	114.80
2	B	401	1E7	C14-N15-C10	2.53	119.91	117.06
2	F	401	1E7	C14-N15-C10	2.47	119.84	117.06
2	G	401	1E7	C3-C23-C24	2.44	122.83	118.53
2	E	401	1E7	C14-N15-C10	2.40	119.76	117.06
2	F	401	1E7	C3-C23-C24	2.37	122.70	118.53
2	D	401	1E7	C14-N15-C10	2.37	119.72	117.06
2	H	401	1E7	C6-C1-N2	2.35	117.63	114.41
2	A	401	1E7	C3-C23-C24	2.28	122.54	118.53
2	H	401	1E7	C14-N15-C10	2.27	119.61	117.06
2	H	401	1E7	C3-C23-C24	2.20	122.40	118.53
2	B	401	1E7	C3-C23-C24	2.03	122.11	118.53
2	E	401	1E7	O31-C27-C3	2.01	117.26	114.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401	1E7	C3-C27-O31-C33
2	F	401	1E7	C26-C27-O31-C33
2	B	401	1E7	C3-C27-O31-C33
2	B	401	1E7	C26-C27-O31-C33

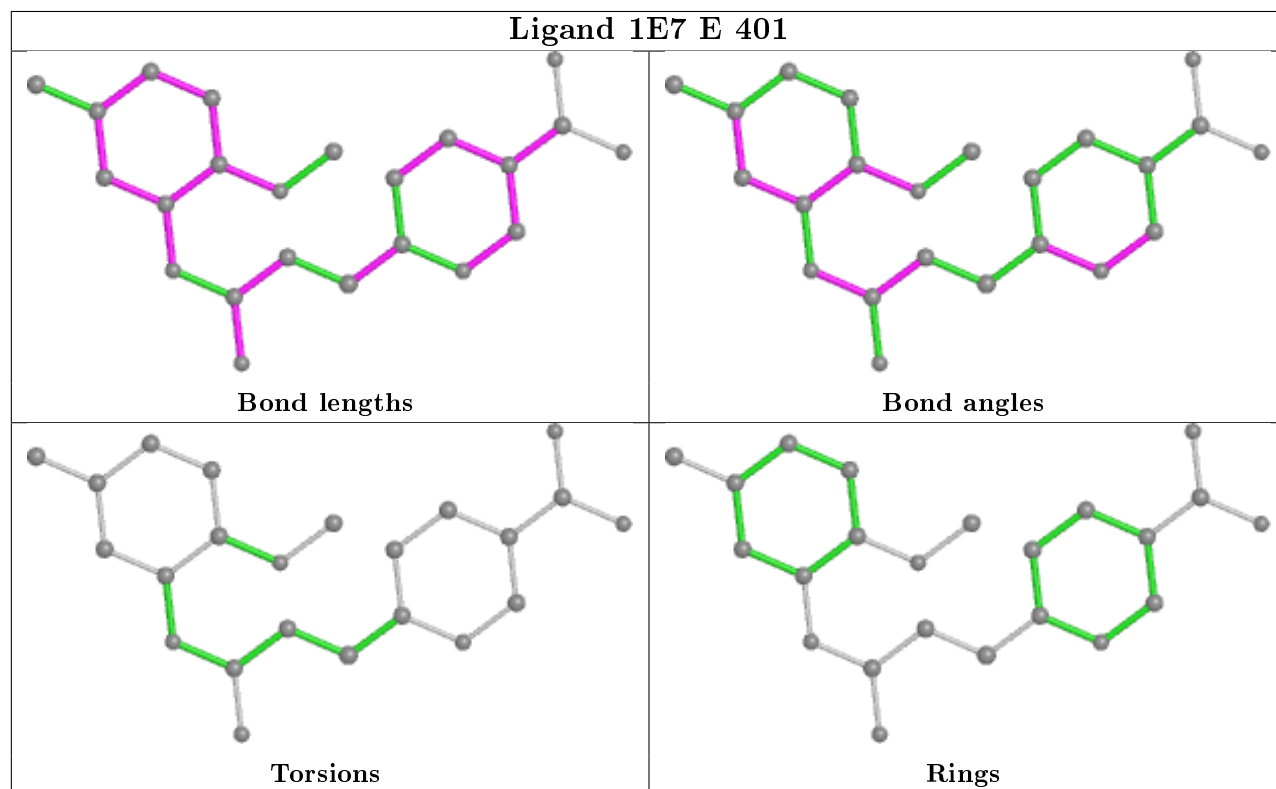
There are no ring outliers.

5 monomers are involved in 5 short contacts:

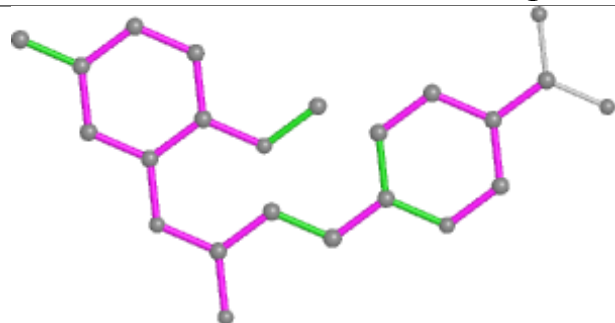
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	1E7	1	0
2	C	401	1E7	1	0
2	B	401	1E7	1	0
2	H	401	1E7	1	0
2	G	401	1E7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

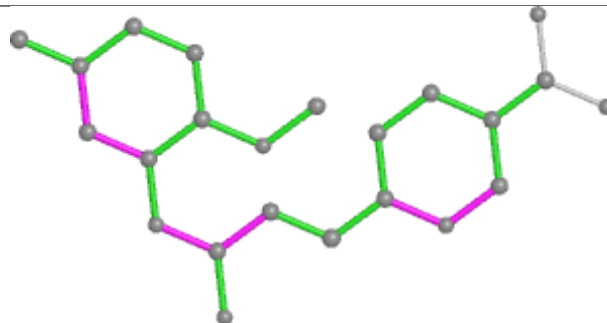
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



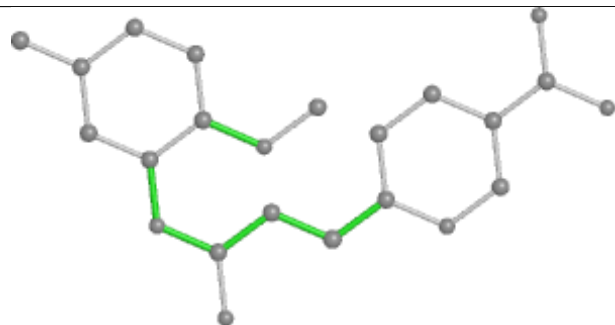
Ligand 1E7 C 401



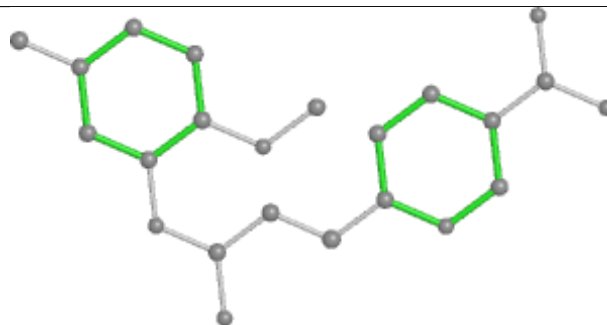
Bond lengths



Bond angles

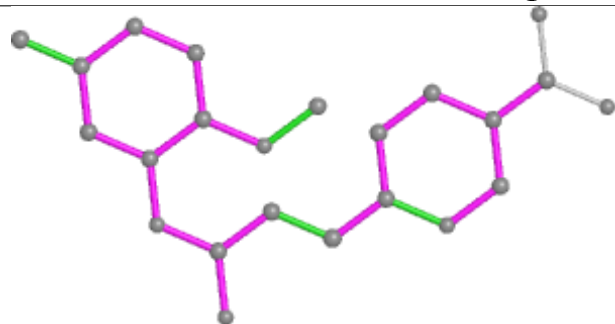


Torsions

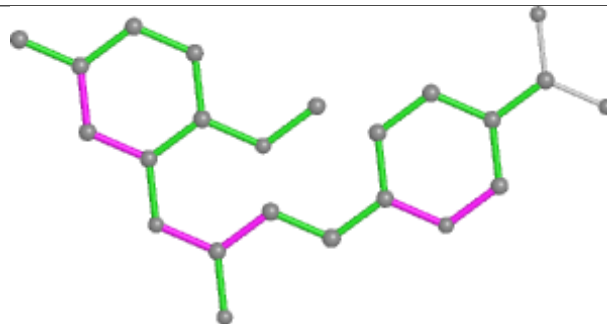


Rings

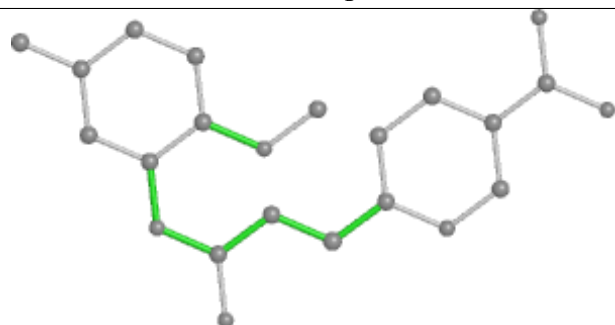
Ligand 1E7 A 401



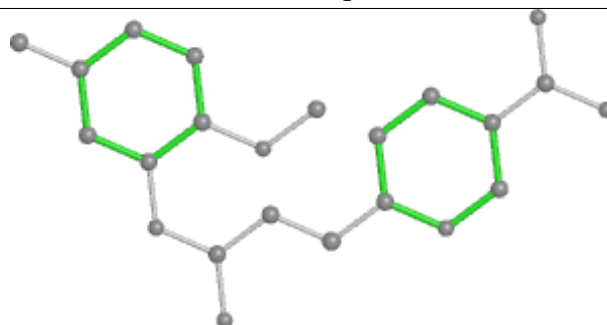
Bond lengths



Bond angles

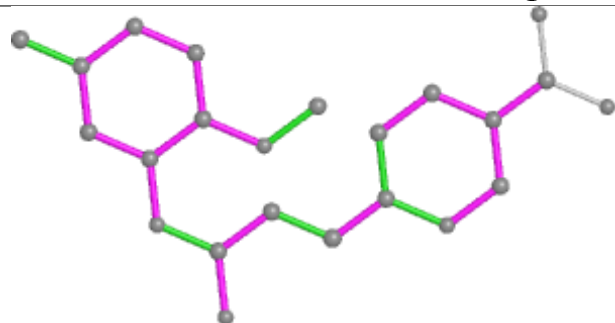


Torsions

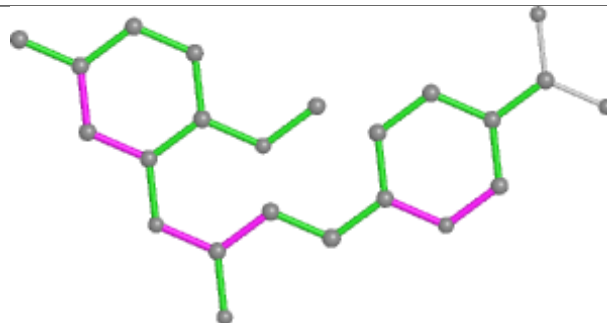


Rings

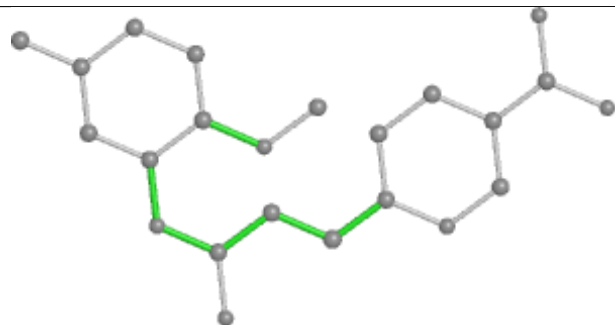
Ligand 1E7 D 401



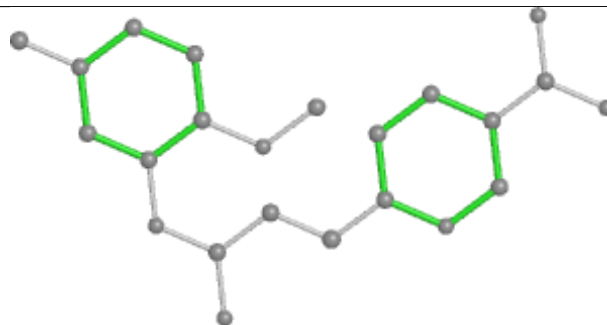
Bond lengths



Bond angles

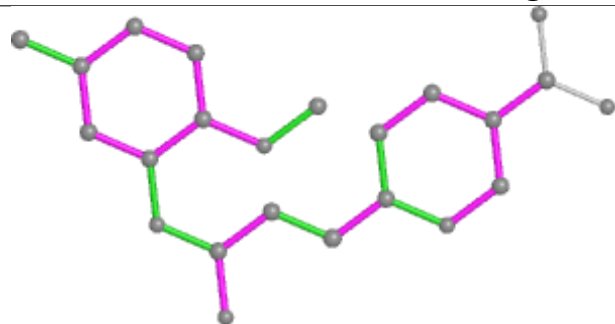


Torsions

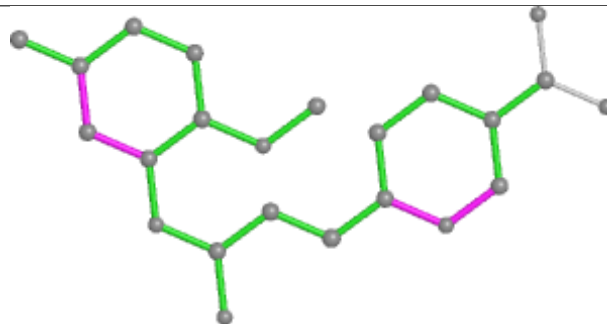


Rings

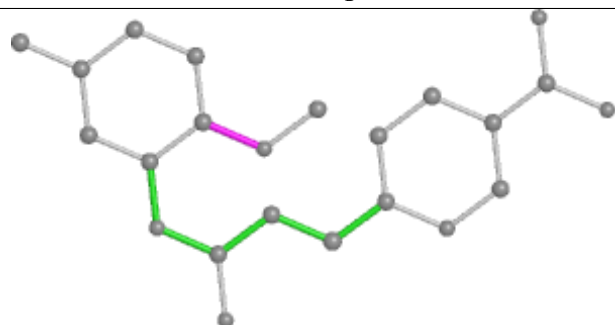
Ligand 1E7 B 401



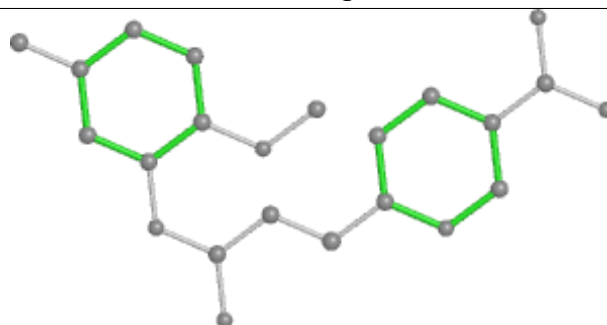
Bond lengths



Bond angles

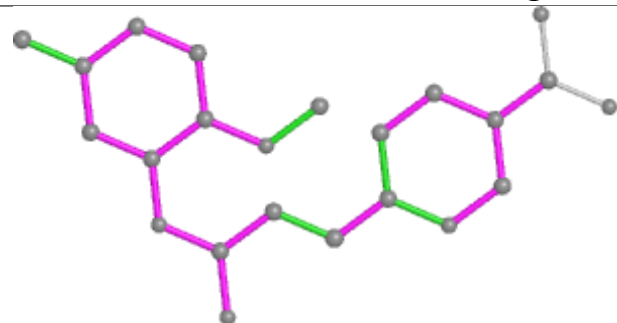


Torsions

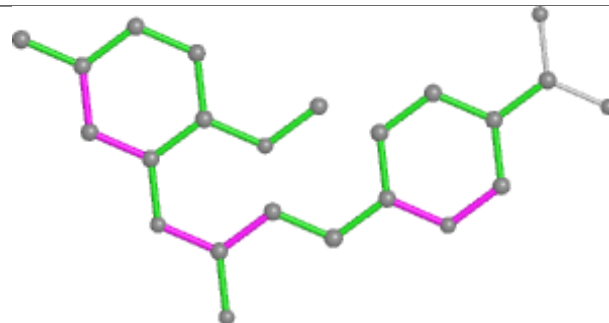


Rings

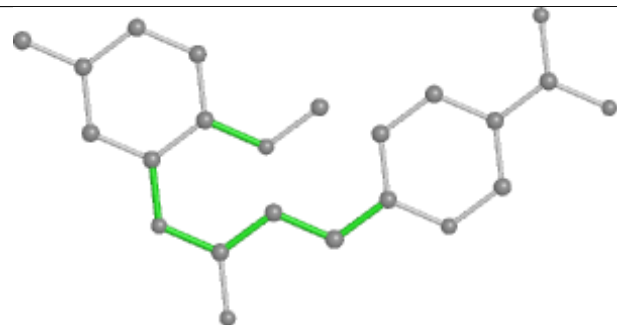
Ligand 1E7 H 401



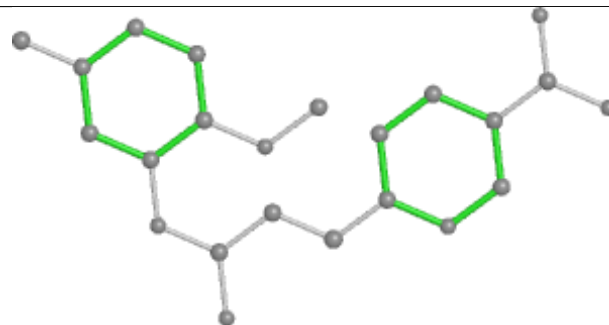
Bond lengths



Bond angles

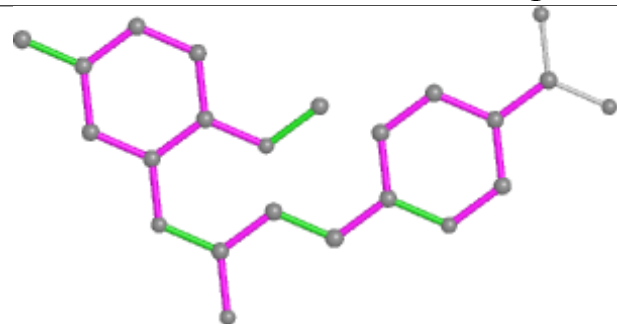


Torsions

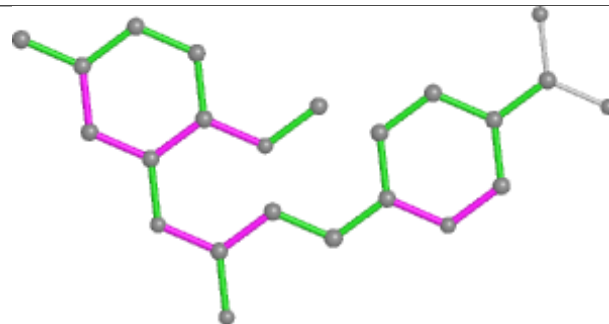


Rings

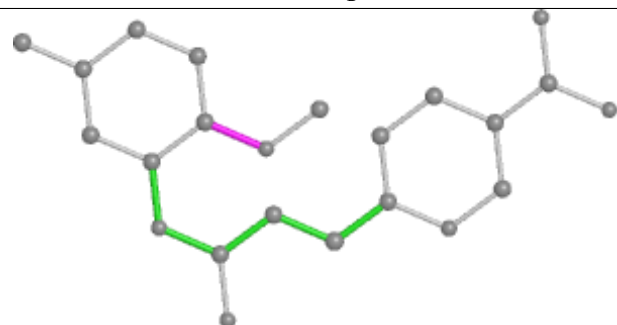
Ligand 1E7 F 401



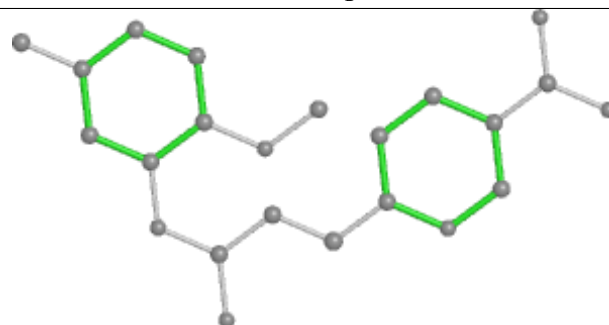
Bond lengths



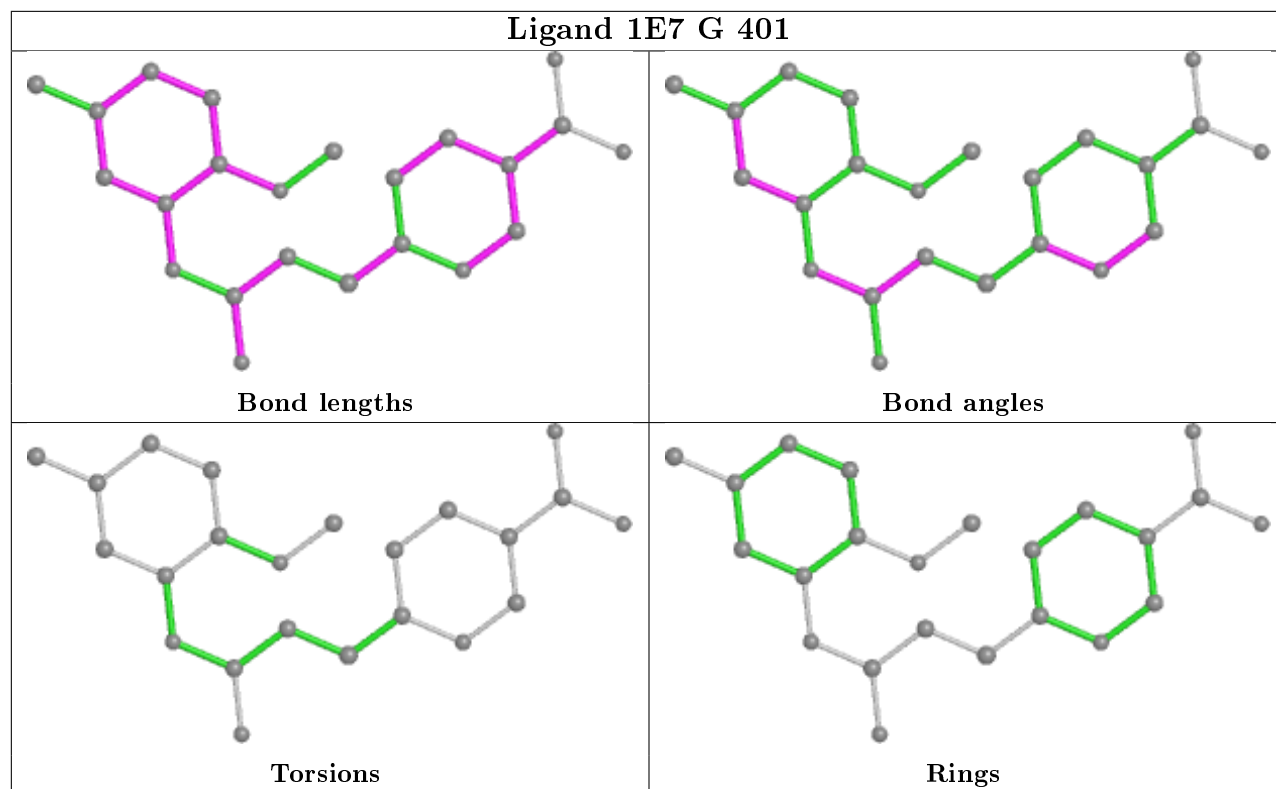
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	323/331 (97%)	-0.20	6 (1%) 66 69	14, 26, 43, 66	1 (0%)
1	B	331/331 (100%)	-0.12	16 (4%) 30 32	13, 25, 50, 88	1 (0%)
1	C	331/331 (100%)	-0.10	10 (3%) 50 53	17, 30, 51, 85	1 (0%)
1	D	331/331 (100%)	-0.16	6 (1%) 68 71	14, 27, 50, 68	1 (0%)
1	E	331/331 (100%)	0.08	10 (3%) 50 53	22, 37, 66, 73	1 (0%)
1	F	329/331 (99%)	0.05	10 (3%) 50 53	20, 34, 64, 78	1 (0%)
1	G	326/331 (98%)	-0.08	12 (3%) 41 45	14, 30, 51, 83	1 (0%)
1	H	326/331 (98%)	-0.08	8 (2%) 57 61	15, 30, 53, 85	1 (0%)
All	All	2628/2648 (99%)	-0.08	78 (2%) 50 53	13, 30, 58, 88	8 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	106	LEU	11.3
1	H	106	LEU	6.3
1	G	106	LEU	6.1
1	H	105	ARG	6.0
1	B	105	ARG	5.7
1	E	15	GLU	4.9
1	B	104	SER	4.7
1	C	102	GLY	4.6
1	G	105	ARG	4.6
1	F	102	GLY	4.3
1	H	12	LEU	4.2
1	B	12	LEU	4.0
1	C	101	GLU	3.9
1	G	97	ALA	3.8
1	F	103	GLU	3.8
1	G	238	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	12	LEU	3.6
1	H	238	TYR	3.5
1	A	14	GLU	3.5
1	B	13	LYS	3.2
1	B	14	GLU	3.2
1	C	100	GLN	3.2
1	G	221	ALA	3.2
1	G	107	ASN	3.2
1	A	16	HIS	3.2
1	A	12	LEU	3.1
1	F	223	LYS	3.1
1	B	99	GLN	3.1
1	H	221	ALA	3.0
1	F	99	GLN	3.0
1	B	100	GLN	2.9
1	D	12	LEU	2.9
1	H	16	HIS	2.9
1	A	98	ARG	2.8
1	G	1	ALA	2.7
1	E	16	HIS	2.7
1	H	97	ALA	2.7
1	E	99	GLN	2.7
1	E	12	LEU	2.7
1	B	238	TYR	2.7
1	C	99	GLN	2.7
1	G	14	GLU	2.6
1	G	104	SER	2.6
1	C	16	HIS	2.6
1	E	309	SER	2.6
1	B	101	GLU	2.5
1	E	105	ARG	2.5
1	A	238	TYR	2.5
1	D	101	GLU	2.5
1	C	238	TYR	2.4
1	F	17	VAL	2.4
1	C	98	ARG	2.3
1	E	13	LYS	2.3
1	F	98	ARG	2.3
1	F	323	TRP	2.2
1	D	15	GLU	2.2
1	D	100	GLN	2.2
1	D	223	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	14	GLU	2.2
1	C	221	ALA	2.1
1	E	310	GLU	2.1
1	H	108	LEU	2.1
1	F	13	LYS	2.1
1	B	1	ALA	2.1
1	D	80	LYS	2.1
1	B	221	ALA	2.1
1	C	52	VAL	2.1
1	B	107	ASN	2.1
1	B	223	LYS	2.1
1	B	16	HIS	2.1
1	F	2	ALA	2.1
1	A	17	VAL	2.1
1	B	98	ARG	2.1
1	E	225	GLN	2.0
1	G	223	LYS	2.0
1	G	52	VAL	2.0
1	F	3	LEU	2.0
1	E	223	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	1E7	E	401	23/23	0.91	0.17	19,32,37,38	0
2	1E7	C	401	23/23	0.91	0.21	17,30,36,40	0
2	1E7	A	401	23/23	0.92	0.23	12,34,43,44	0

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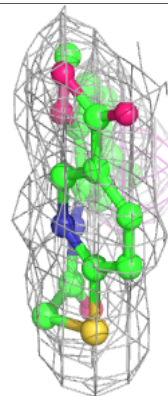
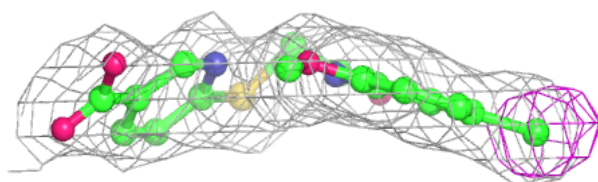
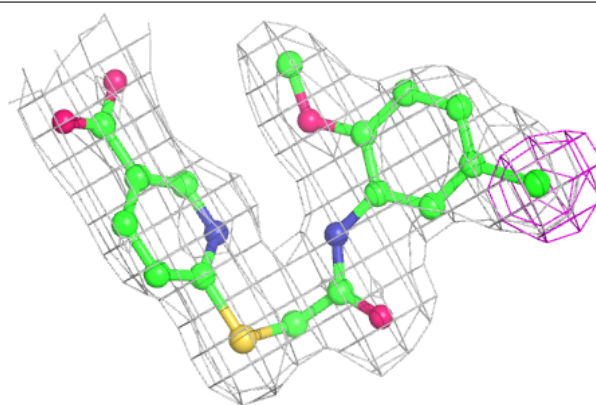
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	1E7	H	401	23/23	0.92	0.23	14,35,41,42	0
2	1E7	F	401	23/23	0.92	0.21	26,39,45,46	0
2	1E7	G	401	23/23	0.92	0.23	28,34,38,41	0
2	1E7	B	401	23/23	0.93	0.19	17,28,31,31	0
2	1E7	D	401	23/23	0.93	0.20	11,27,32,33	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.

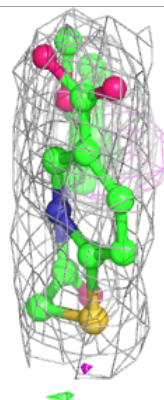
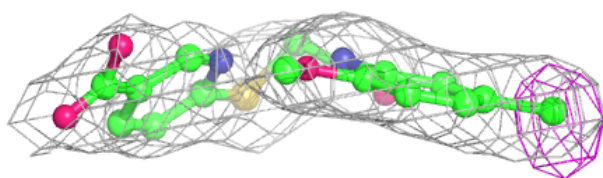
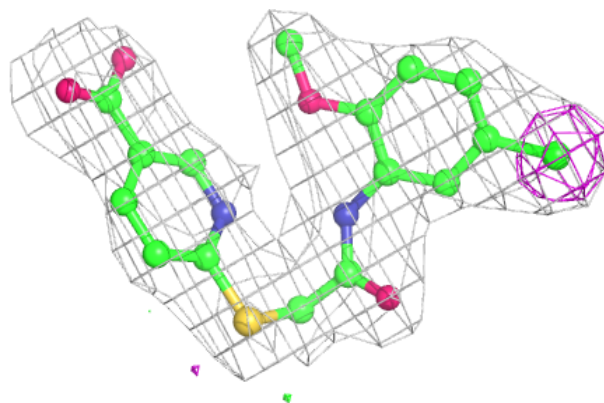
Electron density around 1E7 E 401:

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

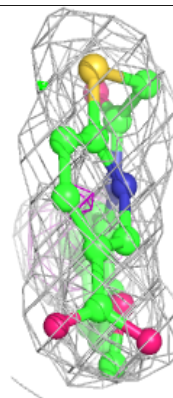
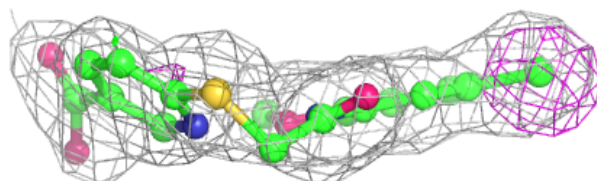
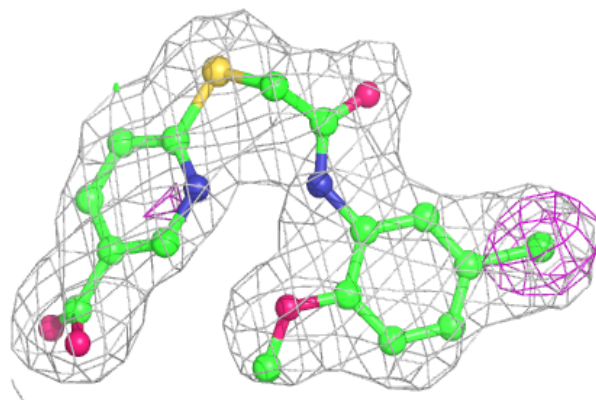


Electron density around 1E7 C 401:

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

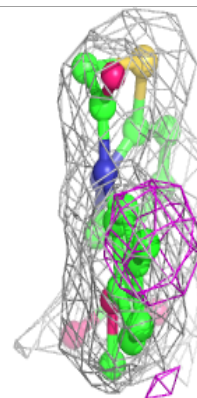
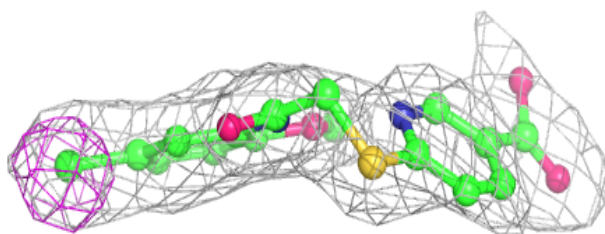
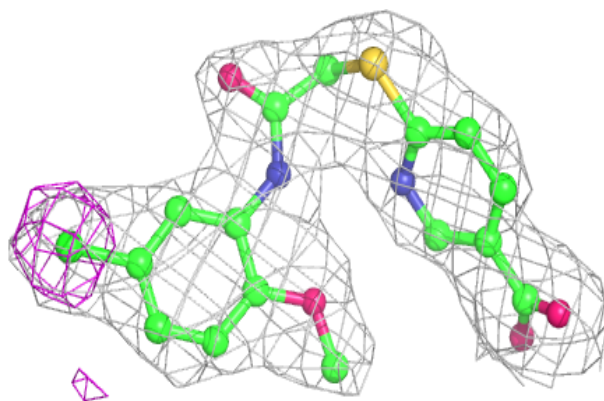
**Electron density around 1E7 A 401:**

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

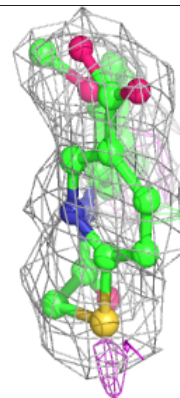
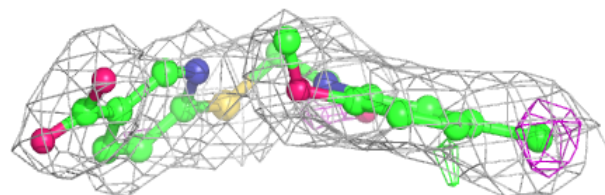
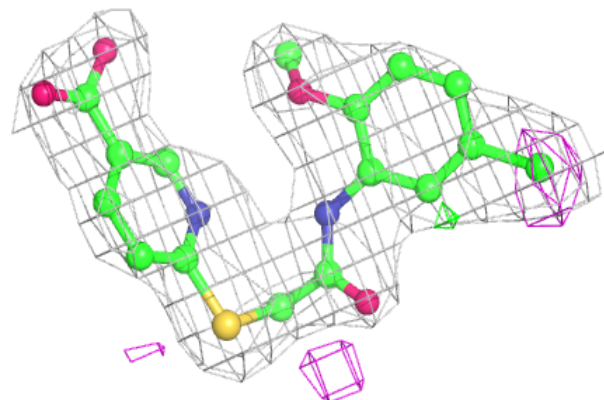


Electron density around 1E7 H 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

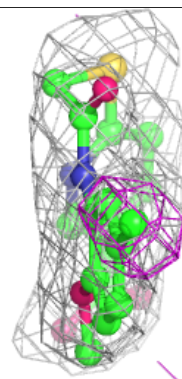
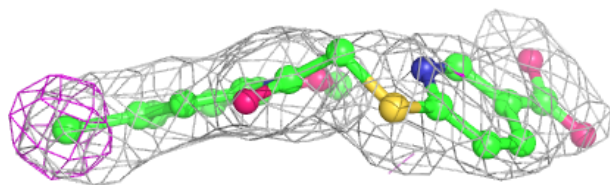
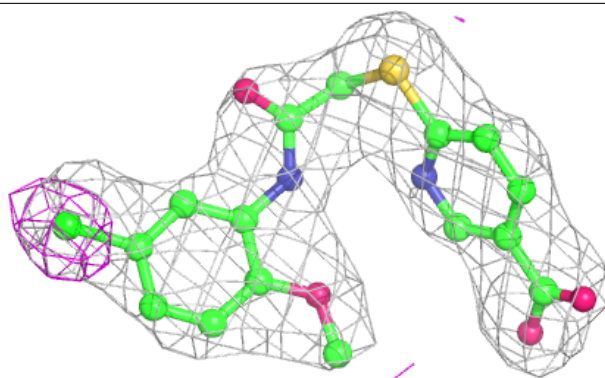
**Electron density around 1E7 F 401:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

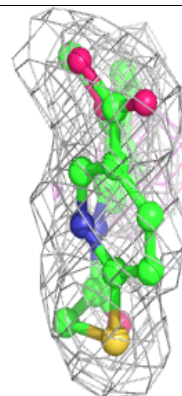
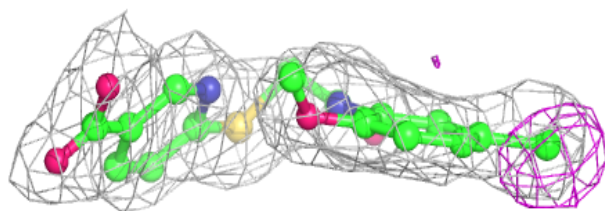
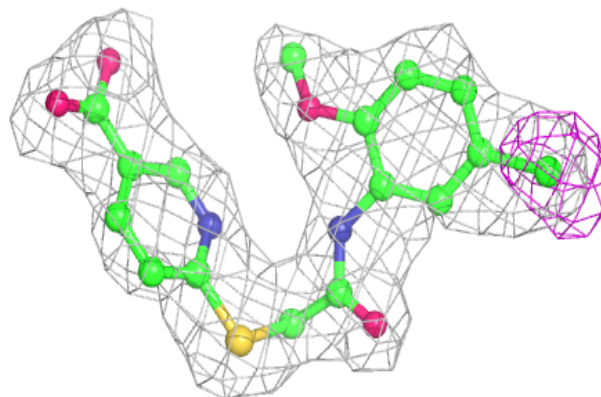


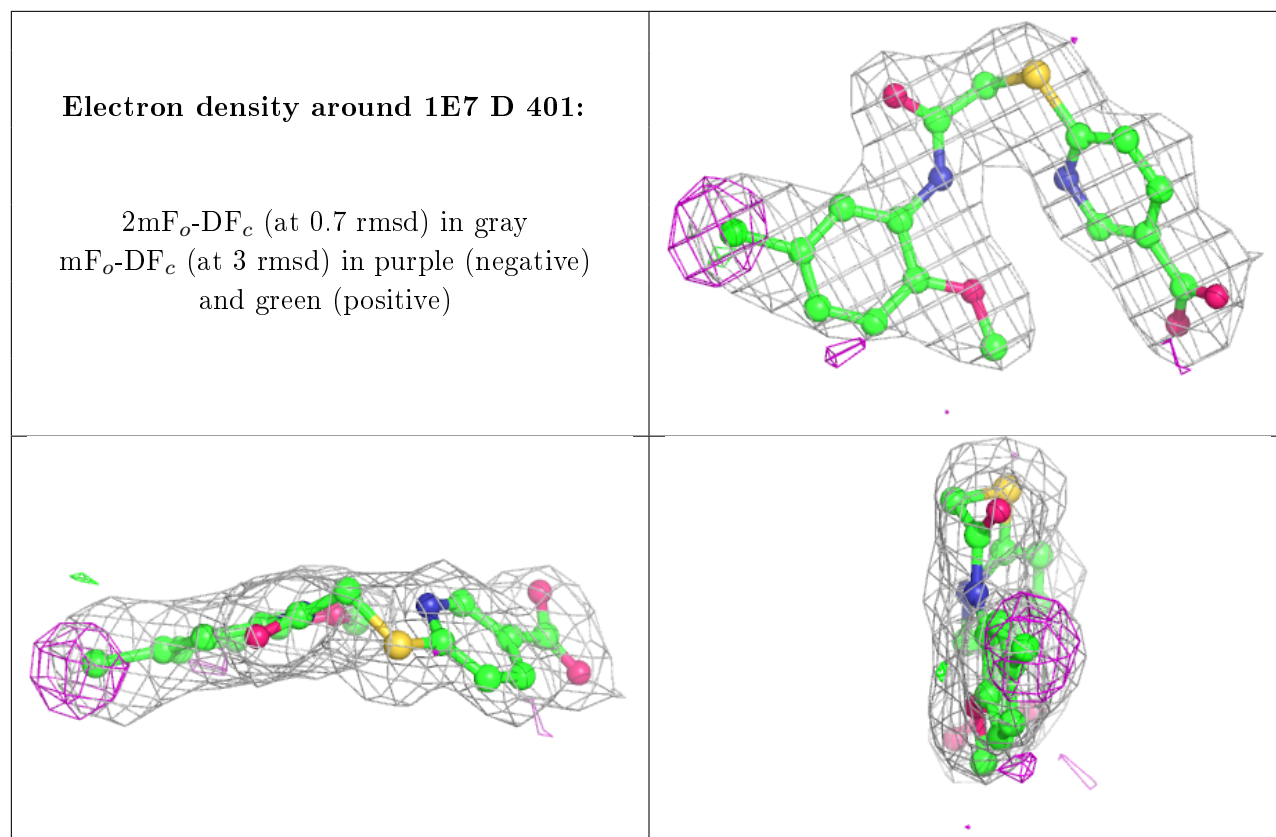
Electron density around 1E7 G 401:

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

**Electron density around 1E7 B 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.