



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:01 AM UTC

PDB ID : 2FIE / pdb_00002fie
Title : Structure of human liver FBPase complexed with potent benzoxazole allosteric inhibitors
Authors : Abad-Zapatero, C.
Deposited on : 2005-12-29
Resolution : 2.81 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

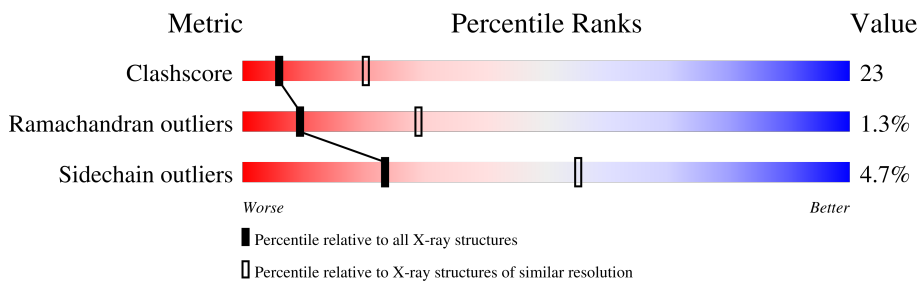
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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))
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	338	
1	D	338	
1	H	338	
1	L	338	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9972 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.

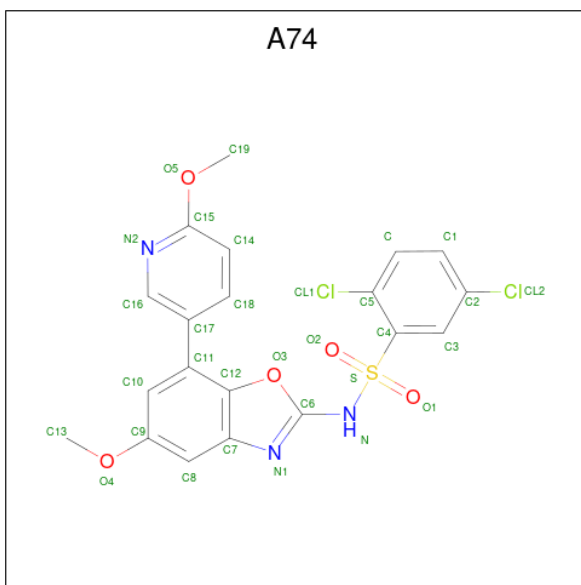
- Molecule 1 is a protein called Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	0	1
			2432	1548	408	459	17			
1	D	319	Total	C	N	O	S	0	0	1
			2432	1548	408	459	17			
1	H	319	Total	C	N	O	S	0	0	1
			2432	1548	408	459	17			
1	L	319	Total	C	N	O	S	0	0	1
			2432	1548	408	459	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	LYS	ARG	variant	GB 15277851
D	217	LYS	ARG	variant	GB 15277851
H	217	LYS	ARG	variant	GB 15277851
L	217	LYS	ARG	variant	GB 15277851

- Molecule 2 is 2,5-DICHLORO-N-[5-METHOXY-7-(6-METHOXPYRIDIN-3-YL)-1,3-BENZOXAZOL-2-YL]BENZENESULFONAMIDE (CCD ID: A74) (formula: C₂₀H₁₅Cl₂N₃O₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 31	C 20	Cl 2	N 3	O 5	S 1	0	0
2	D	1	Total 31	C 20	Cl 2	N 3	O 5	S 1	0	0
2	H	1	Total 31	C 20	Cl 2	N 3	O 5	S 1	0	0
2	L	1	Total 31	C 20	Cl 2	N 3	O 5	S 1	0	0

- Molecule 3 is water.

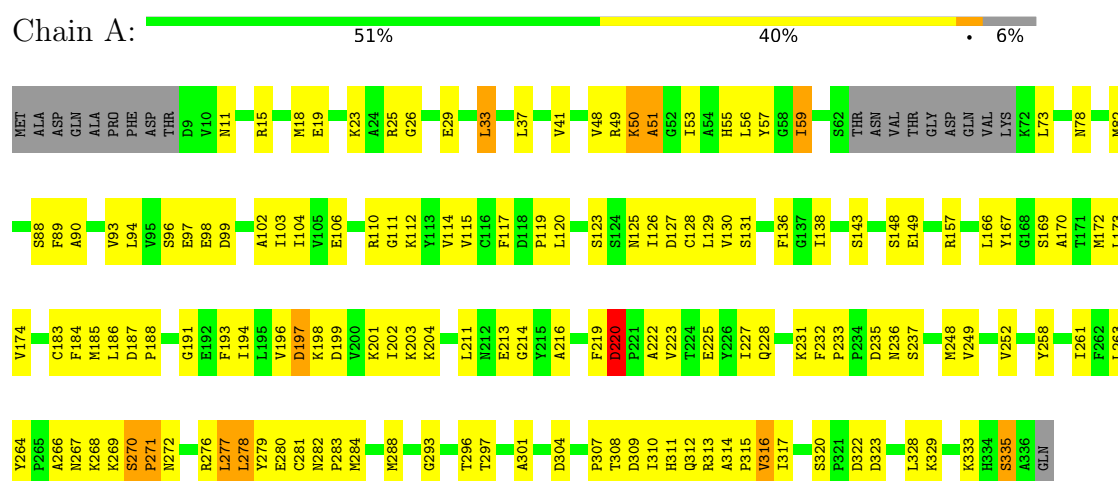
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total	O	0	0
			25	25		
3	D	28	Total	O	0	0
			28	28		
3	H	30	Total	O	0	0
			30	30		
3	L	37	Total	O	0	0
			37	37		

3 Residue-property plots [i](#)

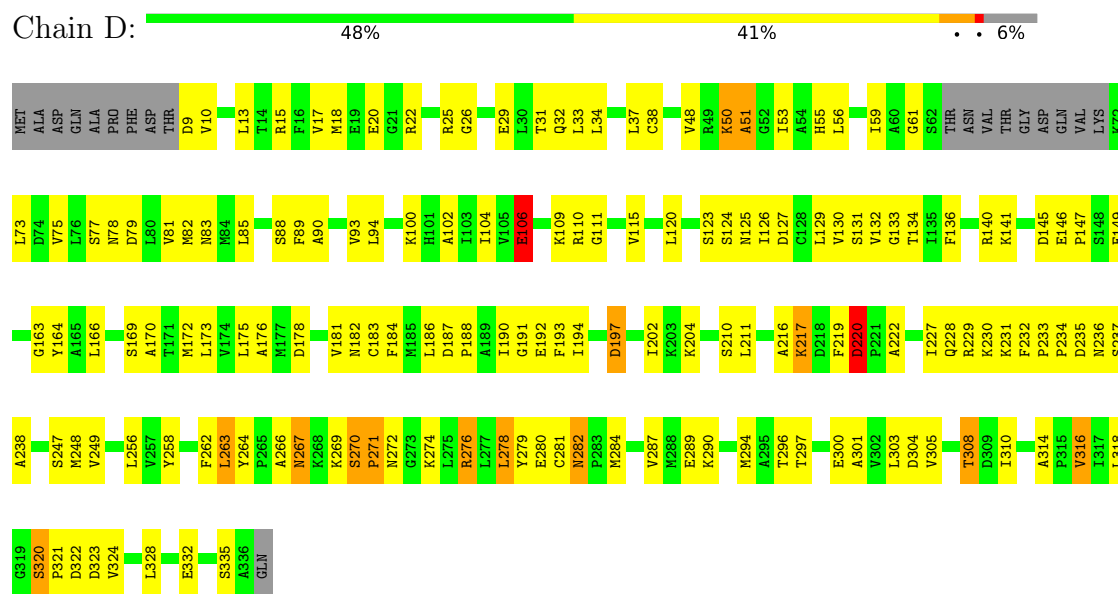
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: Fructose-1,6-bisphosphatase 1

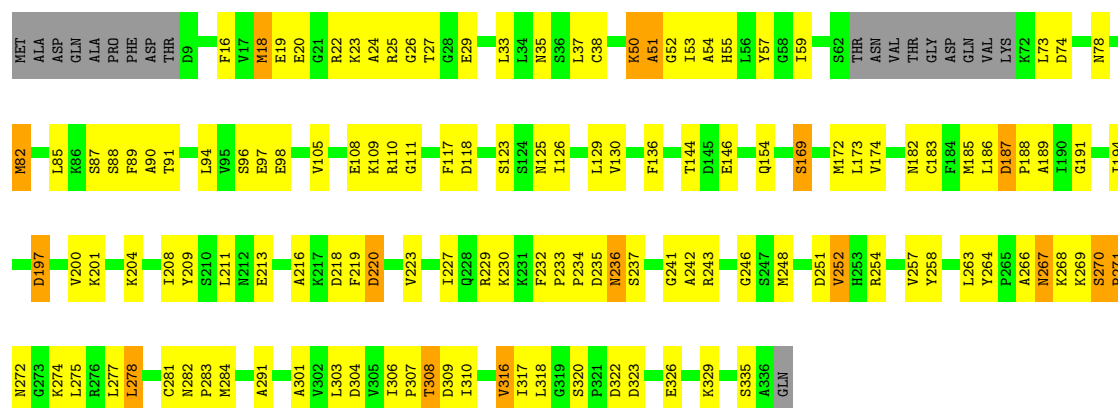


• Molecule 1: Fructose-1,6-bisphosphatase 1



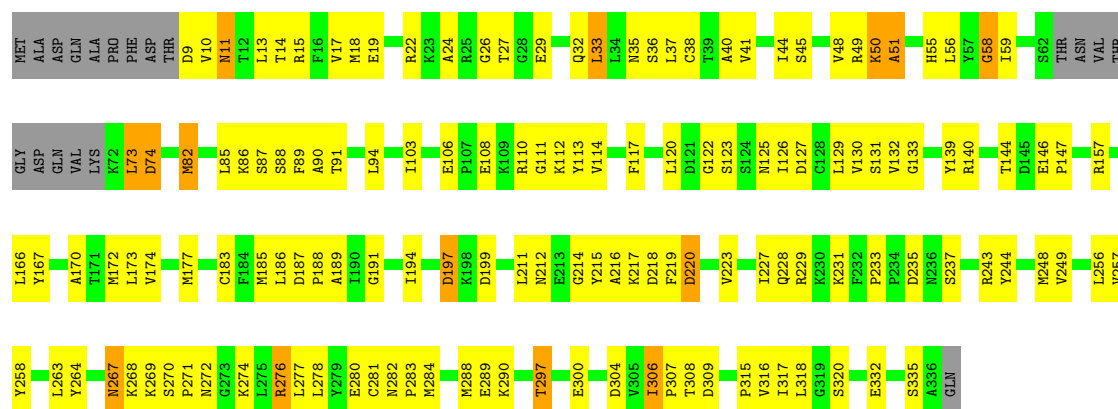
• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain H:  55% 35% 5% 6%



• Molecule 1: Fructose-1,6-bisphosphatase 1

Chain L:  52% 38% 6% 6%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.37Å 83.33Å 277.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.81	Depositor
% Data completeness (in resolution range)	83.7 (19.95-2.81)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.197 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9972	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: A74

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	0.48	1/2475 (0.0%)	1.04	12/3343 (0.4%)
1	D	0.48	1/2475 (0.0%)	1.06	20/3343 (0.6%)
1	H	0.50	1/2475 (0.0%)	1.05	19/3343 (0.6%)
1	L	0.50	1/2475 (0.0%)	1.09	17/3343 (0.5%)
All	All	0.49	4/9900 (0.0%)	1.06	68/13372 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	335	SER	C-N	-5.84	1.25	1.33
1	A	335	SER	C-N	-5.72	1.25	1.33
1	L	335	SER	C-N	-5.60	1.25	1.33
1	D	335	SER	C-N	-5.51	1.25	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	278	LEU	N-CA-C	9.32	121.05	111.07
1	L	264	TYR	CA-C-N	9.14	128.98	120.21
1	L	264	TYR	C-N-CA	9.14	128.98	120.21
1	A	278	LEU	N-CA-C	7.85	119.47	111.07
1	A	214	GLY	N-CA-C	-7.80	104.98	114.66
1	L	306	ILE	CA-C-N	7.54	127.53	119.76
1	L	306	ILE	C-N-CA	7.54	127.53	119.76
1	D	278	LEU	N-CA-C	7.39	119.33	111.28
1	A	233	PRO	CA-C-N	7.32	127.96	119.47
1	A	233	PRO	C-N-CA	7.32	127.96	119.47
1	H	154	GLN	CA-C-N	7.26	127.24	119.76
1	H	154	GLN	C-N-CA	7.26	127.24	119.76
1	H	278	LEU	N-CA-C	7.15	119.94	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	277	LEU	N-CA-C	6.99	119.55	111.02
1	H	306	ILE	N-CA-C	6.64	113.61	107.56
1	L	220	ASP	N-CA-C	-6.51	101.31	110.29
1	L	122	GLY	N-CA-C	-6.50	106.76	115.21
1	H	264	TYR	CA-C-N	6.31	126.76	120.52
1	H	264	TYR	C-N-CA	6.31	126.76	120.52
1	A	277	LEU	N-CA-C	6.30	118.23	111.36
1	A	297	THR	N-CA-C	-6.30	104.90	112.59
1	D	264	TYR	CA-C-N	6.25	127.60	120.85
1	D	264	TYR	C-N-CA	6.25	127.60	120.85
1	L	73	LEU	N-CA-C	-6.23	104.94	112.54
1	H	187	ASP	CA-C-N	6.19	125.88	119.56
1	H	187	ASP	C-N-CA	6.19	125.88	119.56
1	D	238	ALA	CA-C-N	6.17	126.12	119.76
1	D	238	ALA	C-N-CA	6.17	126.12	119.76
1	L	320	SER	CA-C-N	6.17	127.56	119.84
1	L	320	SER	C-N-CA	6.17	127.56	119.84
1	D	308	THR	N-CA-C	-6.13	105.70	113.43
1	H	105	VAL	N-CA-C	6.12	117.64	109.37
1	H	220	ASP	N-CA-C	-6.11	101.15	110.07
1	D	20	GLU	N-CA-C	-5.97	104.35	111.69
1	L	257	VAL	N-CA-C	5.92	116.09	110.53
1	A	264	TYR	CA-C-N	5.89	126.36	120.52
1	A	264	TYR	C-N-CA	5.89	126.36	120.52
1	H	257	VAL	N-CA-C	5.89	115.95	110.42
1	D	110	ARG	N-CA-C	5.88	118.78	109.96
1	H	118	ASP	N-CA-C	-5.78	98.07	109.10
1	H	310	ILE	N-CA-C	5.76	120.11	112.04
1	D	297	THR	N-CA-C	-5.71	106.48	113.50
1	D	100	LYS	N-CA-C	5.67	117.53	111.36
1	A	143	SER	N-CA-C	5.66	117.37	110.41
1	D	314	ALA	CA-C-N	5.56	125.32	119.76
1	D	314	ALA	C-N-CA	5.56	125.32	119.76
1	H	110	ARG	N-CA-C	5.54	118.96	110.20
1	L	117	PHE	N-CA-C	5.49	116.62	108.60
1	H	316	VAL	N-CA-C	5.48	116.55	108.45
1	H	246	GLY	N-CA-C	-5.46	108.20	114.69
1	D	61	GLY	N-CA-C	5.40	122.14	114.85
1	D	320	SER	CA-C-N	5.37	126.56	119.84
1	D	320	SER	C-N-CA	5.37	126.56	119.84
1	L	308	THR	N-CA-C	-5.35	106.81	113.55
1	L	58	GLY	N-CA-C	5.35	123.36	114.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	316	VAL	N-CA-C	5.33	116.34	108.45
1	L	297	THR	N-CA-C	-5.30	106.83	113.72
1	H	169	SER	N-CA-C	-5.29	105.68	111.82
1	A	169	SER	N-CA-C	-5.26	106.37	112.89
1	D	106	GLU	CA-C-N	5.21	125.02	119.28
1	D	106	GLU	C-N-CA	5.21	125.02	119.28
1	A	33	LEU	N-CA-C	-5.15	105.56	111.07
1	H	146	GLU	N-CA-C	-5.13	103.12	109.64
1	L	113	TYR	N-CA-C	5.12	117.74	109.40
1	H	329	LYS	N-CA-C	-5.10	105.61	111.07
1	D	220	ASP	N-CA-C	-5.03	102.84	110.39
1	D	170	ALA	N-CA-C	-5.02	101.66	109.14
1	A	220	ASP	N-CA-C	-5.00	102.88	110.39

There are no chirality outliers.

There are no planarity outliers.

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	2432	0	2474	116	0
1	D	2432	0	2474	132	0
1	H	2432	0	2474	124	0
1	L	2432	0	2474	126	0
2	A	31	0	15	3	0
2	D	31	0	15	4	0
2	H	31	0	15	6	0
2	L	31	0	15	7	0
3	A	25	0	0	2	0
3	D	28	0	0	1	0
3	H	30	0	0	3	0
3	L	37	0	0	3	0
All	All	9972	0	9956	450	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 23.

All (450) 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:H:266:ALA:HB1	1:H:271:PRO:HA	1.36	1.05
1:L:269:LYS:HZ2	1:L:274:LYS:HD2	1.25	0.97
1:A:53:ILE:HA	1:A:56:LEU:HD21	1.53	0.90
1:D:29:GLU:HG3	1:H:22:ARG:HH12	1.39	0.85
1:H:229:ARG:NH1	1:H:234:PRO:HG3	1.94	0.83
1:A:82:MET:HE3	1:A:94:LEU:HD13	1.61	0.82
1:H:129:LEU:HD12	1:L:166:LEU:HD23	1.61	0.82
1:A:106:GLU:O	1:A:110:ARG:HG3	1.80	0.82
1:A:191:GLY:HA3	1:L:191:GLY:HA3	1.63	0.80
1:D:29:GLU:HA	1:H:22:ARG:NH2	1.96	0.80
1:L:82:MET:HE2	1:L:94:LEU:HD13	1.63	0.79
1:A:18:MET:HE2	1:L:18:MET:HE3	1.64	0.79
1:L:269:LYS:NZ	1:L:274:LYS:HD2	1.97	0.78
1:D:125:ASN:O	1:D:130:VAL:HG12	1.84	0.78
1:H:82:MET:HE2	1:H:94:LEU:HD13	1.67	0.77
1:A:26:GLY:CA	2:A:701:A74:HN	1.97	0.77
1:D:29:GLU:HA	1:H:22:ARG:HH22	1.47	0.77
1:D:191:GLY:HA3	1:H:191:GLY:HA3	1.68	0.75
1:D:281:CYS:SG	1:D:316:VAL:HG21	2.27	0.75
1:A:26:GLY:HA3	2:A:701:A74:HN	1.51	0.74
1:A:78:ASN:O	1:A:82:MET:HB2	1.88	0.74
1:H:266:ALA:CB	1:H:271:PRO:HA	2.16	0.74
1:H:183:CYS:HB2	1:H:197:ASP:HB2	1.69	0.74
1:D:266:ALA:HB1	1:D:271:PRO:HA	1.70	0.73
1:D:166:LEU:HD13	1:D:249:VAL:HG12	1.69	0.73
1:H:258:TYR:OH	1:L:127:ASP:HB2	1.87	0.73
1:D:263:LEU:HD12	1:D:263:LEU:N	2.04	0.73
1:D:55:HIS:HA	1:D:59:ILE:HG22	1.71	0.72
1:A:170:ALA:HB3	1:D:129:LEU:HD22	1.72	0.72
1:H:270:SER:C	1:H:272:ASN:H	1.97	0.71
1:L:146:GLU:OE1	1:L:147:PRO:HD2	1.91	0.71
1:H:82:MET:HE2	1:H:94:LEU:CD1	2.21	0.70
1:L:112:LYS:HD2	1:L:140:ARG:CZ	2.20	0.70
1:A:204:LYS:HE2	1:A:322:ASP:OD1	1.91	0.70
1:H:301:ALA:HB3	1:H:304:ASP:OD2	1.92	0.69
1:L:33:LEU:HD23	1:L:90:ALA:HB3	1.73	0.69
1:A:55:HIS:HA	1:A:59:ILE:HG22	1.75	0.68
1:D:230:LYS:HE3	1:D:230:LYS:HA	1.75	0.68
1:A:280:GLU:O	1:A:284:MET:HG2	1.94	0.68
1:A:216:ALA:HA	1:A:219:PHE:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:VAL:HG11	1:H:284:MET:SD	2.34	0.67
1:A:18:MET:CE	1:L:18:MET:HE3	2.24	0.67
1:A:90:ALA:C	1:A:111:GLY:HA3	2.18	0.67
1:A:53:ILE:HA	1:A:56:LEU:CD2	2.24	0.67
1:D:53:ILE:HG13	1:D:56:LEU:HD21	1.77	0.67
1:D:22:ARG:NH2	1:H:29:GLU:HA	2.09	0.67
1:A:173:LEU:C	1:A:173:LEU:HD23	2.20	0.67
1:A:266:ALA:HB1	1:A:271:PRO:HA	1.75	0.67
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.77	0.66
3:H:541:HOH:O	1:L:130:VAL:HA	1.95	0.66
1:D:77:SER:O	1:D:81:VAL:HG23	1.96	0.66
1:D:90:ALA:C	1:D:111:GLY:HA3	2.21	0.65
1:L:316:VAL:C	1:L:317:ILE:HD12	2.20	0.65
1:A:252:VAL:HG21	1:A:284:MET:HE3	1.78	0.65
1:D:88:SER:O	1:D:89:PHE:HB2	1.97	0.65
1:D:53:ILE:HA	1:D:56:LEU:CD2	2.27	0.65
1:H:54:ALA:HB1	1:H:59:ILE:HD12	1.79	0.65
1:A:173:LEU:HD23	1:A:174:VAL:N	2.12	0.64
1:H:316:VAL:C	1:H:317:ILE:HD12	2.23	0.64
1:L:50:LYS:HD2	1:L:50:LYS:N	2.11	0.64
1:D:186:LEU:HB2	1:D:193:PHE:CE1	2.32	0.64
1:A:50:LYS:HD2	1:A:50:LYS:N	2.13	0.64
1:H:108:GLU:H	1:H:108:GLU:CD	2.07	0.63
1:L:112:LYS:HD2	1:L:140:ARG:NH2	2.14	0.62
1:A:227:ILE:HG22	1:A:231:LYS:HE2	1.82	0.62
1:L:133:GLY:HA3	1:L:249:VAL:HG21	1.80	0.62
1:D:229:ARG:NH1	1:D:234:PRO:HG3	2.13	0.62
1:H:204:LYS:HG2	1:H:322:ASP:OD1	1.99	0.62
1:D:270:SER:C	1:D:272:ASN:H	2.07	0.61
1:D:53:ILE:HA	1:D:56:LEU:HD23	1.82	0.61
1:A:82:MET:HE3	1:A:94:LEU:CD1	2.28	0.61
1:D:216:ALA:HA	1:D:219:PHE:CD2	2.35	0.61
1:H:125:ASN:O	1:H:130:VAL:HG12	2.00	0.61
1:A:185:MET:HG2	1:D:53:ILE:HD13	1.82	0.61
1:D:82:MET:HE3	1:D:82:MET:HA	1.82	0.61
1:H:281:CYS:SG	1:H:316:VAL:HG21	2.40	0.61
1:A:172:MET:HG3	1:A:184:PHE:O	2.01	0.60
1:H:270:SER:C	1:H:272:ASN:N	2.59	0.60
1:D:296:THR:HG21	1:D:328:LEU:HD21	1.84	0.60
1:A:127:ASP:HB2	1:D:258:TYR:OH	2.02	0.60
1:D:234:PRO:C	1:D:236:ASN:H	2.09	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:267:ASN:OD1	1:L:268:LYS:N	2.35	0.60
1:A:232:PHE:CE1	1:D:217:LYS:HB2	2.37	0.59
1:H:223:VAL:O	1:H:227:ILE:HG12	2.02	0.59
1:L:82:MET:HE2	1:L:94:LEU:CD1	2.32	0.59
1:H:55:HIS:HA	1:H:59:ILE:HG22	1.83	0.59
1:L:26:GLY:HA3	2:L:1001:A74:HN	1.66	0.59
1:H:201:LYS:HA	1:H:291:ALA:O	2.03	0.59
1:A:213:GLU:HB3	1:D:231:LYS:NZ	2.18	0.59
1:D:106:GLU:OE2	1:D:109:LYS:HD2	2.02	0.59
1:H:35:ASN:O	1:H:38:CYS:HB3	2.02	0.59
1:L:316:VAL:CG1	1:L:318:LEU:HD23	2.33	0.59
1:A:296:THR:HG21	1:A:328:LEU:HD21	1.85	0.58
1:D:26:GLY:CA	2:D:801:A74:HN	2.16	0.58
1:H:216:ALA:HA	1:H:219:PHE:CD2	2.38	0.58
1:L:85:LEU:HD13	1:L:94:LEU:HD22	1.85	0.58
1:A:88:SER:O	1:A:89:PHE:HB2	2.03	0.58
1:D:78:ASN:O	1:D:82:MET:HB2	2.02	0.58
1:A:270:SER:C	1:A:272:ASN:H	2.09	0.58
1:D:281:CYS:SG	1:D:316:VAL:CG2	2.92	0.58
1:D:193:PHE:C	1:D:194:ILE:HD12	2.29	0.58
1:H:209:TYR:CE1	1:H:242:ALA:HB2	2.38	0.58
1:H:50:LYS:HG2	1:L:185:MET:HG2	1.85	0.58
1:H:173:LEU:C	1:H:173:LEU:HD23	2.28	0.58
1:D:73:LEU:HD23	1:D:126:ILE:CD1	2.34	0.58
1:L:317:ILE:HD12	1:L:317:ILE:N	2.19	0.58
1:H:37:LEU:HD21	1:H:136:PHE:CG	2.39	0.57
1:H:26:GLY:CA	2:H:901:A74:HN	2.17	0.57
1:H:317:ILE:HD12	1:H:317:ILE:N	2.19	0.57
1:L:235:ASP:OD2	1:L:237:SER:HB3	2.04	0.57
1:L:270:SER:C	1:L:272:ASN:H	2.13	0.57
1:D:120:LEU:HA	1:D:133:GLY:O	2.05	0.57
1:D:262:PHE:HB3	1:D:318:LEU:HD12	1.87	0.57
1:D:13:LEU:O	1:D:17:VAL:HG23	2.05	0.57
1:D:183:CYS:HB2	1:D:197:ASP:HB2	1.86	0.57
1:L:144:THR:HG22	1:L:144:THR:O	2.04	0.56
1:H:218:ASP:CG	1:H:268:LYS:HB2	2.30	0.56
1:A:276:ARG:O	1:A:280:GLU:HB2	2.05	0.56
1:H:213:GLU:HB3	1:L:231:LYS:NZ	2.20	0.56
1:L:212:ASN:HB2	1:L:244:TYR:CE2	2.40	0.56
1:L:248:MET:HG2	1:L:284:MET:HE3	1.87	0.56
1:A:18:MET:HE2	1:L:18:MET:CE	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:ALA:CB	1:D:149:GLU:HB3	2.36	0.56
1:H:125:ASN:HB2	3:H:536:HOH:O	2.06	0.56
1:H:57:TYR:O	1:L:10:VAL:HB	2.05	0.56
1:D:26:GLY:HA3	2:D:801:A74:HN	1.71	0.55
1:H:16:PHE:CZ	1:H:182:ASN:ND2	2.74	0.55
1:H:229:ARG:HH11	1:H:234:PRO:HG3	1.67	0.55
1:H:251:ASP:OD1	1:H:254:ARG:NH2	2.37	0.55
1:H:24:ALA:HB1	2:H:901:A74:CL1	2.43	0.55
1:L:88:SER:O	1:L:89:PHE:HB2	2.06	0.55
1:D:235:ASP:OD2	1:D:237:SER:HB3	2.05	0.55
1:L:125:ASN:O	1:L:130:VAL:HG12	2.07	0.55
1:H:50:LYS:N	1:H:50:LYS:HD2	2.20	0.55
1:H:233:PRO:HG3	1:H:237:SER:O	2.07	0.55
1:L:183:CYS:HB2	1:L:197:ASP:HB2	1.88	0.55
1:D:228:GLN:HA	1:D:228:GLN:OE1	2.06	0.55
1:L:268:LYS:O	1:L:269:LYS:C	2.50	0.55
1:D:328:LEU:O	1:D:332:GLU:HG3	2.07	0.55
1:H:270:SER:O	1:H:272:ASN:N	2.40	0.55
1:A:187:ASP:OD1	1:D:51:ALA:O	2.25	0.55
1:A:277:LEU:HA	1:A:281:CYS:HB2	1.89	0.55
1:H:37:LEU:HD21	1:H:136:PHE:CD1	2.42	0.55
1:L:22:ARG:HD2	2:L:1001:A74:H133	1.89	0.54
1:D:146:GLU:OE1	1:D:147:PRO:HD2	2.06	0.54
1:D:217:LYS:O	1:D:217:LYS:HG3	2.05	0.54
1:H:90:ALA:HA	1:H:111:GLY:HA3	1.88	0.54
1:A:90:ALA:CA	1:A:111:GLY:HA3	2.37	0.54
1:D:22:ARG:HH22	1:H:29:GLU:HG2	1.71	0.54
1:D:248:MET:HE2	1:D:284:MET:HG3	1.90	0.54
1:D:262:PHE:HB3	1:D:318:LEU:CD1	2.37	0.54
1:L:267:ASN:CG	1:L:268:LYS:H	2.15	0.54
1:A:186:LEU:HB2	1:A:193:PHE:CE1	2.43	0.54
1:L:11:ASN:OD1	1:L:15:ARG:HG2	2.07	0.54
1:A:11:ASN:OD1	1:A:15:ARG:HG2	2.07	0.54
1:H:51:ALA:O	1:L:187:ASP:OD1	2.26	0.54
1:A:98:GLU:HG2	1:A:119:PRO:HG3	1.90	0.54
1:H:85:LEU:HD13	1:H:94:LEU:HD22	1.89	0.54
1:A:19:GLU:HG2	1:L:32:GLN:HE22	1.72	0.53
1:D:94:LEU:CD2	1:D:115:VAL:HB	2.38	0.53
1:L:15:ARG:O	1:L:19:GLU:HG3	2.09	0.53
1:A:267:ASN:OD1	1:A:268:LYS:N	2.41	0.53
1:D:280:GLU:O	1:D:284:MET:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:26:GLY:CA	2:L:1001:A74:HN	2.21	0.53
1:L:41:VAL:HG13	1:L:167:TYR:OH	2.07	0.53
1:D:90:ALA:HA	1:D:111:GLY:HA3	1.90	0.53
1:H:243:ARG:HG2	1:H:243:ARG:HH11	1.74	0.53
1:D:301:ALA:HB3	1:D:304:ASP:OD2	2.08	0.53
1:H:26:GLY:HA3	2:H:901:A74:HN	1.72	0.53
1:L:144:THR:O	1:L:144:THR:CG2	2.56	0.53
1:H:173:LEU:HD23	1:H:174:VAL:N	2.23	0.52
1:H:172:MET:CB	1:L:129:LEU:HD11	2.40	0.52
1:H:200:VAL:HG12	1:H:201:LYS:N	2.23	0.52
1:A:90:ALA:HA	1:A:111:GLY:HA3	1.91	0.52
1:H:187:ASP:OD1	1:H:189:ALA:HB3	2.10	0.52
1:A:220:ASP:OD1	1:A:222:ALA:N	2.39	0.52
1:A:282:ASN:HB2	1:A:283:PRO:HD3	1.92	0.52
1:D:194:ILE:HD12	1:D:194:ILE:N	2.25	0.52
1:D:269:LYS:NZ	1:D:274:LYS:HD2	2.25	0.52
1:D:17:VAL:HG12	1:D:31:THR:HG23	1.92	0.52
1:L:186:LEU:O	1:L:188:PRO:HD3	2.09	0.52
1:L:256:LEU:HD13	1:L:288:MET:HE2	1.92	0.51
1:D:300:GLU:CD	1:D:305:VAL:HG22	2.35	0.51
1:A:97:GLU:HB2	1:A:279:TYR:CE1	2.45	0.51
1:A:102:ALA:HB3	1:A:149:GLU:HG3	1.92	0.51
1:A:276:ARG:NH1	1:A:311:HIS:HB3	2.26	0.51
1:L:33:LEU:HD23	1:L:90:ALA:CB	2.38	0.51
1:A:263:LEU:HG	1:A:317:ILE:HG23	1.92	0.51
1:A:194:ILE:O	1:A:196:VAL:HG13	2.11	0.51
1:A:309:ASP:O	1:A:312:GLN:HB2	2.11	0.51
1:H:194:ILE:HD12	1:H:194:ILE:N	2.25	0.51
1:H:308:THR:HG22	1:H:309:ASP:N	2.25	0.51
1:D:270:SER:O	1:D:272:ASN:N	2.42	0.51
1:D:320:SER:O	1:D:324:VAL:HG23	2.11	0.51
1:L:106:GLU:O	1:L:110:ARG:HG3	2.11	0.51
1:A:93:VAL:HB	1:A:114:VAL:HG13	1.91	0.51
1:A:183:CYS:HB2	1:A:197:ASP:HB2	1.93	0.51
1:D:320:SER:HB2	1:D:323:ASP:OD2	2.11	0.51
1:H:172:MET:HB3	1:L:129:LEU:CD1	2.41	0.51
1:D:289:GLU:OE1	1:D:303:LEU:HD12	2.10	0.51
1:L:24:ALA:HB3	2:L:1001:A74:CL1	2.48	0.51
1:L:13:LEU:HD23	1:L:38:CYS:SG	2.52	0.50
1:L:194:ILE:N	1:L:194:ILE:HD12	2.25	0.50
1:H:169:SER:HB2	1:L:48:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:281:CYS:SG	1:H:316:VAL:CG2	2.99	0.50
1:A:186:LEU:O	1:A:188:PRO:HD3	2.12	0.50
1:H:22:ARG:O	1:H:23:LYS:C	2.53	0.50
1:H:50:LYS:O	1:H:51:ALA:C	2.53	0.50
1:H:90:ALA:C	1:H:111:GLY:HA3	2.37	0.50
1:H:129:LEU:HD11	1:L:172:MET:HB3	1.92	0.50
1:D:90:ALA:CA	1:D:111:GLY:HA3	2.42	0.50
1:L:74:ASP:OD2	1:L:123:SER:HB3	2.12	0.50
1:L:187:ASP:OD1	1:L:189:ALA:HB3	2.11	0.50
1:A:130:VAL:HG22	1:A:131:SER:N	2.27	0.49
1:A:320:SER:HB2	1:A:323:ASP:OD2	2.12	0.49
1:H:269:LYS:NZ	1:H:274:LYS:HG3	2.26	0.49
1:D:172:MET:HG3	1:D:184:PHE:O	2.12	0.49
1:L:33:LEU:HD21	1:L:91:THR:HG23	1.94	0.49
1:A:115:VAL:HG22	1:A:138:ILE:HG12	1.94	0.49
1:H:208:ILE:HA	1:H:241:GLY:O	2.12	0.49
1:L:35:ASN:O	1:L:38:CYS:HB3	2.13	0.49
1:D:18:MET:HE3	1:H:18:MET:CE	2.42	0.49
1:H:318:LEU:HD12	1:H:318:LEU:C	2.38	0.49
1:L:276:ARG:O	1:L:280:GLU:HB2	2.13	0.49
1:A:307:PRO:HA	1:A:312:GLN:OE1	2.11	0.49
1:H:52:GLY:HA2	1:L:187:ASP:OD2	2.12	0.48
1:H:269:LYS:O	1:H:270:SER:CB	2.60	0.48
1:D:102:ALA:HB3	1:D:149:GLU:HB3	1.95	0.48
1:D:73:LEU:HD23	1:D:126:ILE:HD13	1.95	0.48
1:D:75:VAL:HG12	1:D:79:ASP:OD2	2.13	0.48
1:L:120:LEU:HB3	1:L:123:SER:HG	1.77	0.48
1:D:123:SER:O	1:D:124:SER:C	2.56	0.48
1:A:258:TYR:OH	1:D:127:ASP:HB2	2.14	0.48
1:A:270:SER:C	1:A:272:ASN:N	2.72	0.48
1:H:248:MET:CE	1:H:275:LEU:HD13	2.44	0.48
1:H:277:LEU:HA	1:H:281:CYS:HB2	1.95	0.48
1:A:225:GLU:O	1:A:228:GLN:HB2	2.13	0.48
1:D:186:LEU:O	1:D:188:PRO:HD3	2.13	0.48
1:L:14:THR:O	1:L:18:MET:HG3	2.14	0.48
1:A:37:LEU:HD21	1:A:136:PHE:CD2	2.48	0.48
1:D:50:LYS:O	1:D:51:ALA:C	2.57	0.48
1:A:29:GLU:OE1	1:A:112:LYS:HE2	2.14	0.48
1:A:248:MET:HE2	1:A:284:MET:HG3	1.95	0.48
1:L:73:LEU:HD23	1:L:126:ILE:HD13	1.96	0.48
1:L:120:LEU:HB3	1:L:123:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:173:LEU:HD23	1:L:174:VAL:N	2.28	0.48
1:H:19:GLU:O	1:H:20:GLU:C	2.57	0.47
1:H:204:LYS:O	1:H:320:SER:HB3	2.14	0.47
1:A:102:ALA:CB	1:A:149:GLU:HG3	2.44	0.47
1:H:269:LYS:HZ2	1:H:274:LYS:HG3	1.79	0.47
1:L:172:MET:HE3	1:L:185:MET:SD	2.54	0.47
1:D:318:LEU:HD12	1:D:318:LEU:C	2.39	0.47
1:H:282:ASN:HB2	1:H:283:PRO:HD3	1.95	0.47
1:A:57:TYR:O	1:D:10:VAL:HB	2.14	0.47
1:D:22:ARG:HH22	1:H:29:GLU:CG	2.27	0.47
1:H:20:GLU:OE1	1:H:20:GLU:HA	2.14	0.47
1:H:88:SER:O	1:H:89:PHE:HB2	2.14	0.47
1:A:59:ILE:HG12	1:A:59:ILE:O	2.13	0.47
1:A:125:ASN:O	1:A:130:VAL:HG12	2.14	0.47
1:D:85:LEU:HD13	1:D:94:LEU:HD22	1.96	0.47
1:L:316:VAL:HG11	1:L:318:LEU:HD23	1.96	0.47
1:L:282:ASN:HB2	1:L:283:PRO:HD3	1.97	0.47
1:A:281:CYS:SG	1:A:316:VAL:HG11	2.55	0.47
1:A:128:CYS:O	1:A:129:LEU:HB2	2.15	0.47
1:H:22:ARG:CG	2:H:901:A74:H132	2.46	0.46
1:A:104:ILE:HD11	1:A:148:SER:HA	1.96	0.46
1:A:173:LEU:C	1:A:173:LEU:CD2	2.87	0.46
1:A:223:VAL:O	1:A:227:ILE:HG12	2.15	0.46
1:L:40:ALA:O	1:L:44:ILE:HG13	2.15	0.46
1:D:15:ARG:HH12	1:H:87:SER:HB2	1.80	0.46
1:D:134:THR:O	1:D:164:TYR:HA	2.15	0.46
1:D:294:MET:O	1:D:318:LEU:HA	2.15	0.46
1:H:73:LEU:HD23	1:H:126:ILE:CD1	2.45	0.46
1:A:82:MET:SD	1:A:117:PHE:HZ	2.38	0.46
1:L:248:MET:HE2	1:L:284:MET:HG3	1.97	0.46
1:L:276:ARG:NH1	1:L:280:GLU:OE1	2.48	0.46
1:A:235:ASP:OD2	1:A:237:SER:HB3	2.15	0.46
1:D:53:ILE:O	1:D:56:LEU:HD23	2.16	0.46
1:L:211:LEU:HB3	1:L:263:LEU:HB2	1.98	0.46
1:A:276:ARG:NH2	1:A:313:ARG:NH2	2.64	0.46
1:D:202:ILE:HD12	1:D:256:LEU:HA	1.97	0.46
1:H:129:LEU:HD11	1:L:172:MET:CB	2.45	0.46
1:A:19:GLU:O	1:A:23:LYS:HG3	2.15	0.46
1:D:274:LYS:N	3:D:531:HOH:O	2.49	0.46
1:D:34:LEU:O	1:D:37:LEU:HB3	2.15	0.45
1:D:173:LEU:HD23	1:D:173:LEU:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ILE:HG13	1:D:192:GLU:HB2	1.99	0.45
1:L:37:LEU:O	1:L:41:VAL:HG23	2.15	0.45
1:A:170:ALA:HB3	1:D:129:LEU:CD2	2.45	0.45
1:A:172:MET:SD	1:A:183:CYS:HB3	2.56	0.45
1:D:25:ARG:HA	2:D:801:A74:C18	2.47	0.45
1:D:140:ARG:HG3	1:D:141:LYS:N	2.29	0.45
1:H:186:LEU:O	1:H:188:PRO:HD3	2.15	0.45
1:L:297:THR:HG22	1:L:315:PRO:O	2.16	0.45
1:A:278:LEU:HD23	1:A:278:LEU:HA	1.74	0.45
1:D:48:VAL:HA	1:D:73:LEU:HD21	1.97	0.45
1:L:177:MET:HE1	2:L:1001:A74:CL2	2.53	0.45
1:D:130:VAL:HG22	1:D:131:SER:N	2.30	0.45
1:L:17:VAL:HG13	2:L:1001:A74:CL2	2.53	0.45
1:D:102:ALA:HB2	1:D:149:GLU:HB3	1.98	0.45
1:H:235:ASP:OD2	1:H:237:SER:HB3	2.17	0.45
1:A:56:LEU:H	1:A:56:LEU:HD23	1.80	0.45
1:D:210:SER:O	1:D:263:LEU:HD12	2.16	0.45
1:L:218:ASP:O	1:L:267:ASN:HB2	2.16	0.45
1:A:48:VAL:C	1:A:50:LYS:H	2.24	0.45
1:A:252:VAL:CG2	1:A:284:MET:HE3	2.46	0.45
1:D:234:PRO:C	1:D:236:ASN:N	2.75	0.45
1:H:89:PHE:CE2	1:H:109:LYS:HG2	2.52	0.45
1:H:172:MET:HB2	1:L:129:LEU:HD11	1.99	0.45
1:A:15:ARG:NH2	1:L:87:SER:HB2	2.32	0.45
1:L:120:LEU:O	1:L:123:SER:OG	2.30	0.45
1:A:25:ARG:HA	2:A:701:A74:C18	2.46	0.45
1:A:235:ASP:O	1:A:237:SER:N	2.49	0.45
1:H:229:ARG:NH2	1:H:326:GLU:OE2	2.50	0.45
1:H:243:ARG:HG2	1:H:243:ARG:NH1	2.31	0.45
1:L:157:ARG:HH21	1:L:304:ASP:CG	2.25	0.45
1:A:106:GLU:HG3	3:A:585:HOH:O	2.17	0.45
1:A:41:VAL:HG13	1:A:167:TYR:OH	2.17	0.44
1:D:270:SER:C	1:D:272:ASN:N	2.73	0.44
1:H:22:ARG:HG2	2:H:901:A74:H132	1.99	0.44
1:H:263:LEU:HD12	1:H:263:LEU:N	2.32	0.44
1:L:223:VAL:O	1:L:227:ILE:HG12	2.17	0.44
1:A:51:ALA:O	1:D:187:ASP:OD1	2.35	0.44
1:A:276:ARG:HH11	1:A:311:HIS:HB3	1.81	0.44
1:D:204:LYS:O	1:D:320:SER:HB3	2.17	0.44
1:A:103:ILE:N	1:A:103:ILE:HD12	2.33	0.44
1:L:50:LYS:O	1:L:51:ALA:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ILE:HG12	1:A:203:LYS:N	2.32	0.44
1:A:288:MET:O	1:A:293:GLY:N	2.51	0.44
1:D:269:LYS:O	1:D:270:SER:CB	2.66	0.44
1:D:276:ARG:HG2	1:D:279:TYR:CZ	2.53	0.44
1:H:129:LEU:HD22	1:L:170:ALA:HB3	1.99	0.44
1:A:301:ALA:HB3	1:A:304:ASP:OD2	2.17	0.44
1:D:13:LEU:HD23	1:D:38:CYS:SG	2.58	0.44
1:H:123:SER:O	1:H:126:ILE:HG22	2.18	0.44
1:D:125:ASN:O	1:D:130:VAL:CG1	2.63	0.44
1:H:96:SER:HA	1:H:117:PHE:O	2.18	0.44
1:L:36:SER:OG	1:L:88:SER:HB3	2.17	0.44
1:A:261:ILE:HD11	1:A:317:ILE:CG2	2.48	0.44
1:H:220:ASP:OD2	1:H:223:VAL:HG23	2.17	0.44
1:A:172:MET:HG2	1:A:173:LEU:N	2.33	0.43
1:D:247:SER:O	1:D:248:MET:C	2.61	0.43
1:L:214:GLY:C	1:L:216:ALA:H	2.26	0.43
1:L:229:ARG:O	1:L:233:PRO:HA	2.18	0.43
1:L:290:LYS:HA	1:L:290:LYS:HD3	1.86	0.43
1:A:96:SER:HB3	1:A:99:ASP:OD2	2.18	0.43
1:A:269:LYS:O	1:A:270:SER:OG	2.33	0.43
1:D:93:VAL:HG22	1:D:104:ILE:CD1	2.47	0.43
1:L:73:LEU:HD23	1:L:126:ILE:CD1	2.48	0.43
1:L:82:MET:O	1:L:86:LYS:HG3	2.18	0.43
1:A:120:LEU:HD23	1:A:123:SER:OG	2.18	0.43
1:H:25:ARG:HA	2:H:901:A74:C18	2.48	0.43
1:A:49:ARG:NH1	1:D:169:SER:O	2.49	0.43
1:H:232:PHE:HE1	1:L:217:LYS:HA	1.84	0.43
1:H:267:ASN:OD1	1:H:268:LYS:N	2.51	0.43
1:H:282:ASN:HD22	1:H:282:ASN:HA	1.67	0.43
1:L:55:HIS:HA	1:L:59:ILE:HG22	2.00	0.43
1:L:300:GLU:HB2	3:L:552:HOH:O	2.18	0.43
1:L:49:ARG:O	1:L:50:LYS:HB2	2.18	0.43
1:L:256:LEU:HD13	1:L:288:MET:CE	2.48	0.43
1:L:270:SER:HA	1:L:271:PRO:HD3	1.82	0.43
1:L:29:GLU:HB2	3:L:516:HOH:O	2.18	0.43
1:L:157:ARG:NH1	1:L:289:GLU:OE1	2.51	0.43
1:A:136:PHE:CD1	1:A:136:PHE:C	2.96	0.43
1:L:33:LEU:HD21	1:L:91:THR:CG2	2.49	0.43
1:D:318:LEU:HD12	1:D:318:LEU:O	2.19	0.43
1:H:78:ASN:O	1:H:82:MET:HB2	2.19	0.43
1:L:33:LEU:HD13	1:L:33:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:136:PHE:CZ	1:D:163:GLY:HA3	2.54	0.43
1:D:248:MET:O	1:D:249:VAL:C	2.60	0.43
1:H:320:SER:HB2	1:H:323:ASP:OD2	2.19	0.43
1:L:306:ILE:HA	1:L:307:PRO:HD3	1.75	0.43
1:A:37:LEU:HD21	1:A:136:PHE:CG	2.54	0.42
1:D:83:ASN:ND2	1:L:58:GLY:O	2.52	0.42
1:D:93:VAL:HG22	1:D:104:ILE:HD12	2.00	0.42
1:D:175:LEU:HD12	1:D:176:ALA:N	2.34	0.42
1:D:176:ALA:HB2	1:D:287:VAL:HG22	2.00	0.42
1:L:82:MET:HG3	1:L:86:LYS:HE3	2.01	0.42
1:L:112:LYS:HB2	1:L:140:ARG:NH1	2.34	0.42
1:L:114:VAL:HB	1:L:139:TYR:HB2	2.01	0.42
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.86	0.42
1:D:276:ARG:O	1:D:280:GLU:HB2	2.19	0.42
1:H:278:LEU:HD21	1:H:307:PRO:CG	2.50	0.42
1:D:204:LYS:HG2	1:D:322:ASP:OD1	2.20	0.42
1:A:329:LYS:HB3	1:A:329:LYS:HE2	1.74	0.42
1:L:45:SER:O	1:L:49:ARG:HD3	2.19	0.42
1:L:108:GLU:CD	1:L:108:GLU:H	2.27	0.42
1:A:184:PHE:HB3	1:A:193:PHE:HB3	2.00	0.42
1:A:73:LEU:HD23	1:A:126:ILE:CD1	2.49	0.42
1:D:282:ASN:HD22	1:D:282:ASN:HA	1.63	0.42
1:H:230:LYS:HD2	1:H:230:LYS:N	2.34	0.42
1:L:126:ILE:HG12	1:L:126:ILE:O	2.20	0.42
1:L:228:GLN:OE1	1:L:228:GLN:HA	2.20	0.42
1:A:104:ILE:CD1	1:A:148:SER:HA	2.50	0.42
1:A:129:LEU:HD11	1:D:172:MET:HB2	2.01	0.42
1:D:32:GLN:OE1	1:H:22:ARG:NH2	2.53	0.42
1:D:278:LEU:CD1	1:D:310:ILE:HA	2.49	0.42
1:D:320:SER:HA	1:D:321:PRO:HD3	1.89	0.42
1:L:90:ALA:C	1:L:111:GLY:HA3	2.45	0.42
1:H:97:GLU:O	1:H:97:GLU:HG2	2.19	0.42
1:D:17:VAL:HG13	2:D:801:A74:CL2	2.57	0.41
1:H:29:GLU:HB2	3:H:616:HOH:O	2.20	0.41
1:L:33:LEU:CD2	1:L:90:ALA:HB3	2.46	0.41
2:L:1001:A74:O3	2:L:1001:A74:H18	2.19	0.41
1:A:198:LYS:O	1:A:199:ASP:C	2.62	0.41
1:D:29:GLU:CG	1:H:22:ARG:HH12	2.19	0.41
1:D:38:CYS:HG	1:D:193:PHE:HD2	1.66	0.41
1:H:272:ASN:HD22	1:H:272:ASN:HA	1.65	0.41
1:A:166:LEU:HD23	1:D:129:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:ILE:HD13	1:D:227:ILE:HA	1.89	0.41
1:H:90:ALA:CA	1:H:111:GLY:HA3	2.51	0.41
1:H:248:MET:HE3	1:H:275:LEU:HD13	2.01	0.41
1:D:290:LYS:HD3	1:D:290:LYS:HA	1.86	0.41
1:L:243:ARG:HG2	1:L:243:ARG:HH11	1.86	0.41
1:H:96:SER:C	1:H:98:GLU:N	2.77	0.41
1:H:173:LEU:C	1:H:173:LEU:CD2	2.92	0.41
1:L:130:VAL:HG22	1:L:131:SER:N	2.36	0.41
1:L:268:LYS:C	1:L:270:SER:N	2.76	0.41
1:L:280:GLU:O	1:L:284:MET:HG2	2.19	0.41
1:A:248:MET:HG2	1:A:284:MET:HE2	2.02	0.41
1:D:220:ASP:OD1	1:D:222:ALA:N	2.51	0.41
1:L:281:CYS:SG	1:L:316:VAL:HG21	2.61	0.41
1:A:314:ALA:HA	1:A:315:PRO:HD3	1.90	0.41
1:D:296:THR:OG1	1:D:300:GLU:O	2.36	0.41
1:H:89:PHE:CD2	1:H:109:LYS:HA	2.55	0.41
1:H:200:VAL:CG1	1:H:201:LYS:N	2.83	0.41
1:L:103:ILE:HD12	1:L:103:ILE:N	2.35	0.41
1:D:181:VAL:HG12	1:D:182:ASN:N	2.35	0.41
1:H:125:ASN:HA	1:L:258:TYR:OH	2.21	0.41
1:H:130:VAL:HA	3:L:513:HOH:O	2.20	0.41
1:H:282:ASN:HD22	1:H:303:LEU:HD23	1.86	0.41
1:L:173:LEU:HD23	1:L:173:LEU:C	2.46	0.41
1:A:203:LYS:HG3	3:A:524:HOH:O	2.21	0.41
1:L:216:ALA:HA	1:L:219:PHE:CD2	2.56	0.41
1:A:157:ARG:HA	1:A:157:ARG:HD3	1.86	0.40
1:H:185:MET:HG2	1:L:50:LYS:HG2	2.03	0.40
1:L:146:GLU:OE1	1:L:146:GLU:HA	2.21	0.40
1:A:278:LEU:HD12	1:A:310:ILE:HA	2.03	0.40
1:D:232:PHE:O	1:D:233:PRO:C	2.63	0.40
1:H:50:LYS:HG3	1:H:53:ILE:HD12	2.02	0.40
1:L:82:MET:HA	1:L:82:MET:HE3	2.02	0.40
1:D:230:LYS:N	1:D:230:LYS:HD2	2.35	0.40
1:H:33:LEU:CD2	1:H:91:THR:HG23	2.52	0.40
1:D:37:LEU:HD21	1:D:136:PHE:CG	2.56	0.40
1:D:48:VAL:C	1:D:50:LYS:H	2.29	0.40
1:H:53:ILE:HG22	1:L:187:ASP:HB2	2.04	0.40
1:H:97:GLU:O	1:H:97:GLU:CG	2.69	0.40
1:H:318:LEU:HD12	1:H:318:LEU:O	2.22	0.40
1:A:333:LYS:O	1:A:333:LYS:HG2	2.22	0.40
1:D:266:ALA:O	1:D:267:ASN:HB3	2.21	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	315/338 (93%)	289 (92%)	22 (7%)	4 (1%)	9	29
1	D	315/338 (93%)	284 (90%)	27 (9%)	4 (1%)	9	29
1	H	315/338 (93%)	287 (91%)	23 (7%)	5 (2%)	7	24
1	L	315/338 (93%)	289 (92%)	22 (7%)	4 (1%)	9	29
All	All	1260/1352 (93%)	1149 (91%)	94 (8%)	17 (1%)	9	29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	D	51	ALA
1	D	267	ASN
1	D	270	SER
1	H	51	ALA
1	H	270	SER
1	H	236	ASN
1	L	51	ALA
1	A	51	ALA
1	H	267	ASN
1	L	215	TYR
1	L	199	ASP
1	L	267	ASN
1	A	270	SER
1	D	271	PRO
1	H	271	PRO
1	A	271	PRO

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	265/281 (94%)	255 (96%)	10 (4%)	29	62
1	D	265/281 (94%)	250 (94%)	15 (6%)	18	47
1	H	265/281 (94%)	254 (96%)	11 (4%)	26	59
1	L	265/281 (94%)	251 (95%)	14 (5%)	20	50
All	All	1060/1124 (94%)	1010 (95%)	50 (5%)	23	55

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	50	LYS
1	A	59	ILE
1	A	197	ASP
1	A	201	LYS
1	A	211	LEU
1	A	220	ASP
1	A	308	THR
1	A	316	VAL
1	A	335	SER
1	D	9	ASP
1	D	33	LEU
1	D	50	LYS
1	D	106	GLU
1	D	132	VAL
1	D	145	ASP
1	D	178	ASP
1	D	197	ASP
1	D	211	LEU
1	D	217	LYS
1	D	220	ASP
1	D	263	LEU
1	D	276	ARG
1	D	282	ASN

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Mol	Chain	Res	Type
1	D	308	THR
1	H	18	MET
1	H	27	THR
1	H	50	LYS
1	H	74	ASP
1	H	82	MET
1	H	144	THR
1	H	197	ASP
1	H	211	LEU
1	H	236	ASN
1	H	252	VAL
1	H	308	THR
1	L	9	ASP
1	L	11	ASN
1	L	27	THR
1	L	33	LEU
1	L	50	LYS
1	L	56	LEU
1	L	74	ASP
1	L	82	MET
1	L	132	VAL
1	L	197	ASP
1	L	220	ASP
1	L	276	ARG
1	L	309	ASP
1	L	332	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	A	154	GLN
1	A	158	ASN
1	A	272	ASN
1	A	282	ASN
1	D	11	ASN
1	D	35	ASN
1	D	154	GLN
1	D	182	ASN
1	D	272	ASN
1	D	282	ASN
1	H	35	ASN

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Mol	Chain	Res	Type
1	H	101	HIS
1	H	272	ASN
1	H	282	ASN
1	L	35	ASN
1	L	125	ASN
1	L	272	ASN
1	L	282	ASN
1	L	334	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](#)

4 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	A74	D	801	-	34,34,34	2.85	17 (50%)	47,50,50	1.47	10 (21%)
2	A74	A	701	-	34,34,34	2.54	17 (50%)	47,50,50	1.52	7 (14%)
2	A74	L	1001	-	34,34,34	2.42	15 (44%)	47,50,50	1.54	9 (19%)
2	A74	H	901	-	34,34,34	2.96	20 (58%)	47,50,50	1.64	8 (17%)

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	A74	D	801	-	-	8/17/19/19	0/4/4/4
2	A74	A	701	-	-	6/17/19/19	0/4/4/4
2	A74	L	1001	-	-	6/17/19/19	0/4/4/4
2	A74	H	901	-	-	8/17/19/19	0/4/4/4

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	A74	C6-N	7.06	1.49	1.36
2	H	901	A74	C6-N	6.80	1.49	1.36
2	A	701	A74	C6-N	6.72	1.49	1.36
2	L	1001	A74	C6-N	6.47	1.48	1.36
2	D	801	A74	C12-C7	5.57	1.43	1.38
2	A	701	A74	C6-N1	5.51	1.39	1.30
2	H	901	A74	C6-N1	5.44	1.39	1.30
2	D	801	A74	C11-C12	5.37	1.50	1.41
2	H	901	A74	C11-C12	5.06	1.50	1.41
2	L	1001	A74	C11-C12	5.03	1.50	1.41
2	H	901	A74	C15-N2	5.03	1.40	1.32
2	L	1001	A74	C6-N1	4.87	1.38	1.30
2	D	801	A74	C6-N1	4.70	1.38	1.30
2	H	901	A74	C12-C7	4.69	1.42	1.38
2	A	701	A74	C11-C12	4.62	1.49	1.41
2	L	1001	A74	C15-N2	4.30	1.39	1.32
2	H	901	A74	C11-C17	4.23	1.57	1.49
2	H	901	A74	C10-C9	4.10	1.45	1.39
2	D	801	A74	C11-C17	3.84	1.56	1.49
2	D	801	A74	C3-C2	3.80	1.44	1.38
2	D	801	A74	C15-N2	3.75	1.38	1.32
2	H	901	A74	O5-C15	3.68	1.41	1.35
2	A	701	A74	C5-C4	3.56	1.44	1.40
2	L	1001	A74	C10-C9	3.36	1.44	1.39
2	D	801	A74	C3-C4	3.33	1.44	1.39
2	D	801	A74	O5-C15	3.27	1.40	1.35
2	H	901	A74	C16-N2	3.13	1.40	1.34
2	A	701	A74	C8-C9	3.11	1.44	1.39
2	D	801	A74	C18-C14	3.10	1.43	1.38
2	H	901	A74	C3-C2	3.06	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	A74	C15-N2	2.96	1.37	1.32
2	H	901	A74	C3-C4	2.85	1.43	1.39
2	H	901	A74	C8-C9	2.85	1.43	1.39
2	A	701	A74	O4-C9	2.83	1.43	1.37
2	L	1001	A74	O4-C9	2.81	1.43	1.37
2	A	701	A74	C10-C9	2.80	1.43	1.39
2	H	901	A74	C5-C4	2.77	1.43	1.40
2	L	1001	A74	O5-C15	2.76	1.39	1.35
2	D	801	A74	C-C5	2.74	1.44	1.38
2	H	901	A74	C1-C	2.66	1.43	1.38
2	A	701	A74	C1-C	2.65	1.43	1.38
2	L	1001	A74	C1-C	2.65	1.43	1.38
2	D	801	A74	C8-C9	2.64	1.43	1.39
2	D	801	A74	C10-C9	2.62	1.43	1.39
2	A	701	A74	C3-C4	2.58	1.43	1.39
2	A	701	A74	O3-C12	-2.58	1.34	1.38
2	H	901	A74	C18-C17	2.56	1.44	1.39
2	H	901	A74	O3-C12	-2.52	1.34	1.38
2	L	1001	A74	C8-C9	2.49	1.43	1.39
2	H	901	A74	C16-C17	2.48	1.43	1.39
2	A	701	A74	C3-C2	2.44	1.42	1.38
2	A	701	A74	C12-C7	2.44	1.40	1.38
2	L	1001	A74	C3-C4	2.42	1.43	1.39
2	A	701	A74	O5-C15	2.39	1.39	1.35
2	A	701	A74	C1-C2	2.36	1.42	1.38
2	H	901	A74	C4-S	2.28	1.80	1.77
2	A	701	A74	C11-C17	2.25	1.53	1.49
2	L	1001	A74	C1-C2	2.24	1.42	1.38
2	D	801	A74	C16-C17	2.23	1.43	1.39
2	L	1001	A74	C10-C11	2.23	1.43	1.39
2	L	1001	A74	C5-C4	2.23	1.43	1.40
2	H	901	A74	O4-C9	2.20	1.41	1.37
2	H	901	A74	C-C5	2.20	1.43	1.38
2	A	701	A74	C-C5	2.13	1.43	1.38
2	L	1001	A74	C16-C17	2.11	1.43	1.39
2	D	801	A74	C18-C17	2.08	1.43	1.39
2	D	801	A74	O3-C12	-2.07	1.35	1.38
2	D	801	A74	C1-C	2.04	1.42	1.38
2	L	1001	A74	C3-C2	2.03	1.41	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	901	A74	C4-S-N	6.30	113.80	105.96
2	L	1001	A74	C8-C7-C12	4.49	124.39	120.81
2	D	801	A74	C8-C7-C12	4.39	124.31	120.81
2	A	701	A74	C16-N2-C15	4.23	120.56	116.72
2	H	901	A74	C8-C7-C12	3.95	123.96	120.81
2	A	701	A74	C8-C7-C12	3.84	123.87	120.81
2	A	701	A74	C4-S-N	3.77	110.65	105.96
2	L	1001	A74	C4-S-N	3.75	110.62	105.96
2	D	801	A74	O3-C12-C11	3.33	132.49	125.93
2	D	801	A74	C4-S-N	3.29	110.05	105.96
2	L	1001	A74	C16-N2-C15	3.21	119.64	116.72
2	D	801	A74	C16-N2-C15	3.13	119.57	116.72
2	L	1001	A74	O3-C12-C7	3.13	111.13	107.69
2	A	701	A74	O3-C12-C7	3.07	111.07	107.69
2	H	901	A74	C16-N2-C15	3.01	119.46	116.72
2	H	901	A74	O3-C12-C11	2.75	131.35	125.93
2	L	1001	A74	O3-C12-C11	2.74	131.34	125.93
2	L	1001	A74	C19-O5-C15	-2.71	113.30	117.33
2	L	1001	A74	O2-S-O1	-2.69	116.26	119.52
2	H	901	A74	O3-C12-C7	2.59	110.54	107.69
2	A	701	A74	O3-C12-C11	2.54	130.94	125.93
2	D	801	A74	O2-S-O1	-2.52	116.46	119.52
2	A	701	A74	C14-C15-N2	-2.41	120.89	124.65
2	A	701	A74	C19-O5-C15	-2.38	113.78	117.33
2	D	801	A74	C14-C15-N2	-2.31	121.04	124.65
2	H	901	A74	C4-C5-CL1	2.30	123.18	121.52
2	H	901	A74	C14-C15-N2	-2.28	121.09	124.65
2	H	901	A74	O2-S-O1	-2.22	116.83	119.52
2	D	801	A74	C18-C17-C11	2.21	124.56	120.91
2	D	801	A74	C11-C10-C9	2.18	123.22	119.84
2	L	1001	A74	C14-C15-N2	-2.17	121.26	124.65
2	D	801	A74	O3-C12-C7	2.10	110.00	107.69
2	L	1001	A74	O3-C6-N1	-2.08	111.84	115.57
2	D	801	A74	C19-O5-C15	-2.07	114.25	117.33

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	A74	C10-C11-C17-C16
2	A	701	A74	C12-C11-C17-C16
2	D	801	A74	C10-C11-C17-C16
2	D	801	A74	C12-C11-C17-C16

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Mol	Chain	Res	Type	Atoms
2	H	901	A74	C10-C11-C17-C16
2	H	901	A74	C12-C11-C17-C16
2	H	901	A74	C14-C15-O5-C19
2	H	901	A74	N2-C15-O5-C19
2	L	1001	A74	C10-C11-C17-C16
2	L	1001	A74	C12-C11-C17-C16
2	H	901	A74	C10-C9-O4-C13
2	D	801	A74	C10-C11-C17-C18
2	H	901	A74	C8-C9-O4-C13
2	H	901	A74	C10-C11-C17-C18
2	L	1001	A74	C10-C11-C17-C18
2	A	701	A74	C10-C11-C17-C18
2	H	901	A74	C12-C11-C17-C18
2	L	1001	A74	C12-C11-C17-C18
2	A	701	A74	C12-C11-C17-C18
2	D	801	A74	C12-C11-C17-C18
2	D	801	A74	C10-C9-O4-C13
2	A	701	A74	C14-C15-O5-C19
2	D	801	A74	C14-C15-O5-C19
2	A	701	A74	N2-C15-O5-C19
2	D	801	A74	C8-C9-O4-C13
2	D	801	A74	N2-C15-O5-C19
2	L	1001	A74	N2-C15-O5-C19
2	L	1001	A74	C14-C15-O5-C19

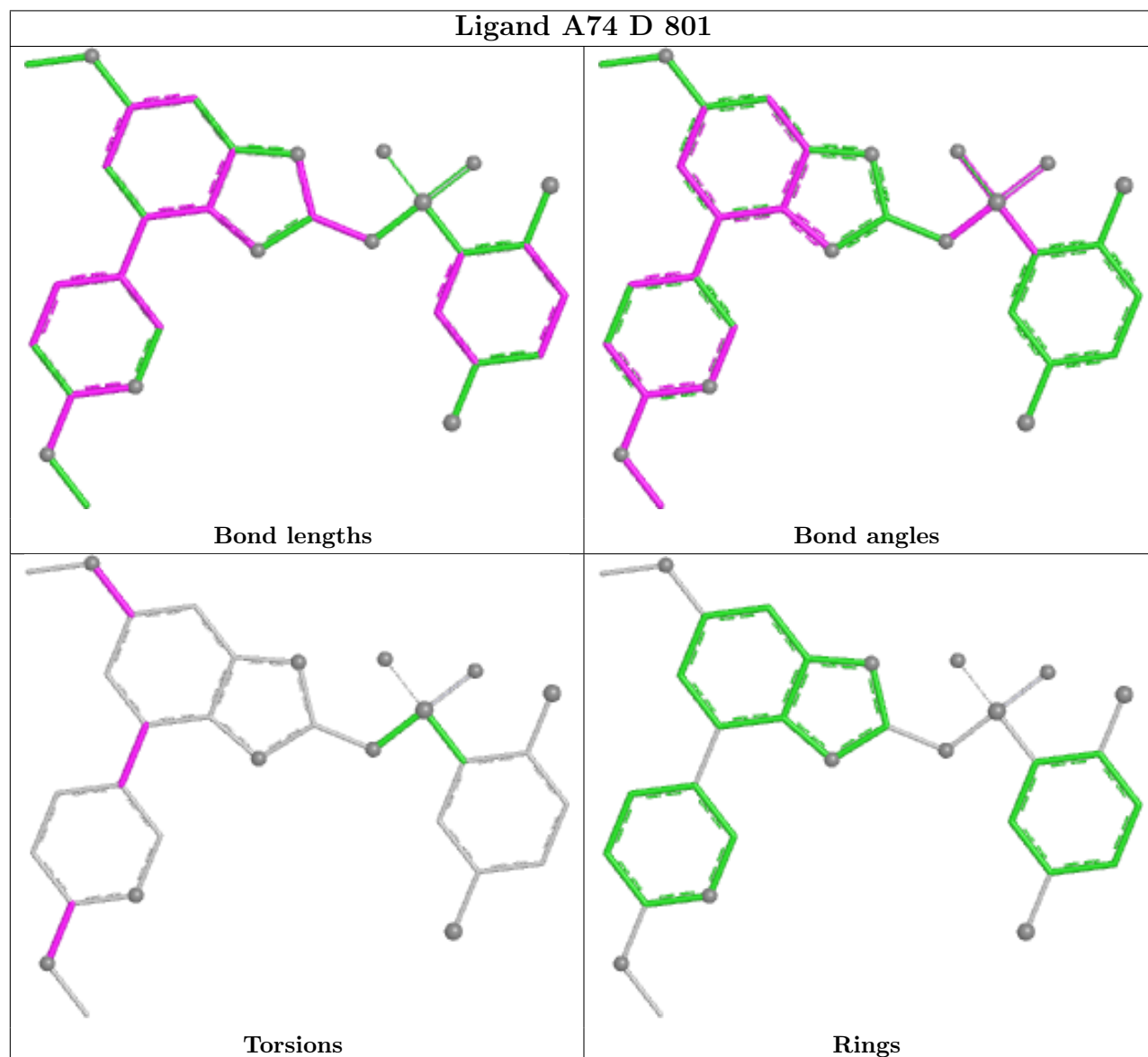
There are no ring outliers.

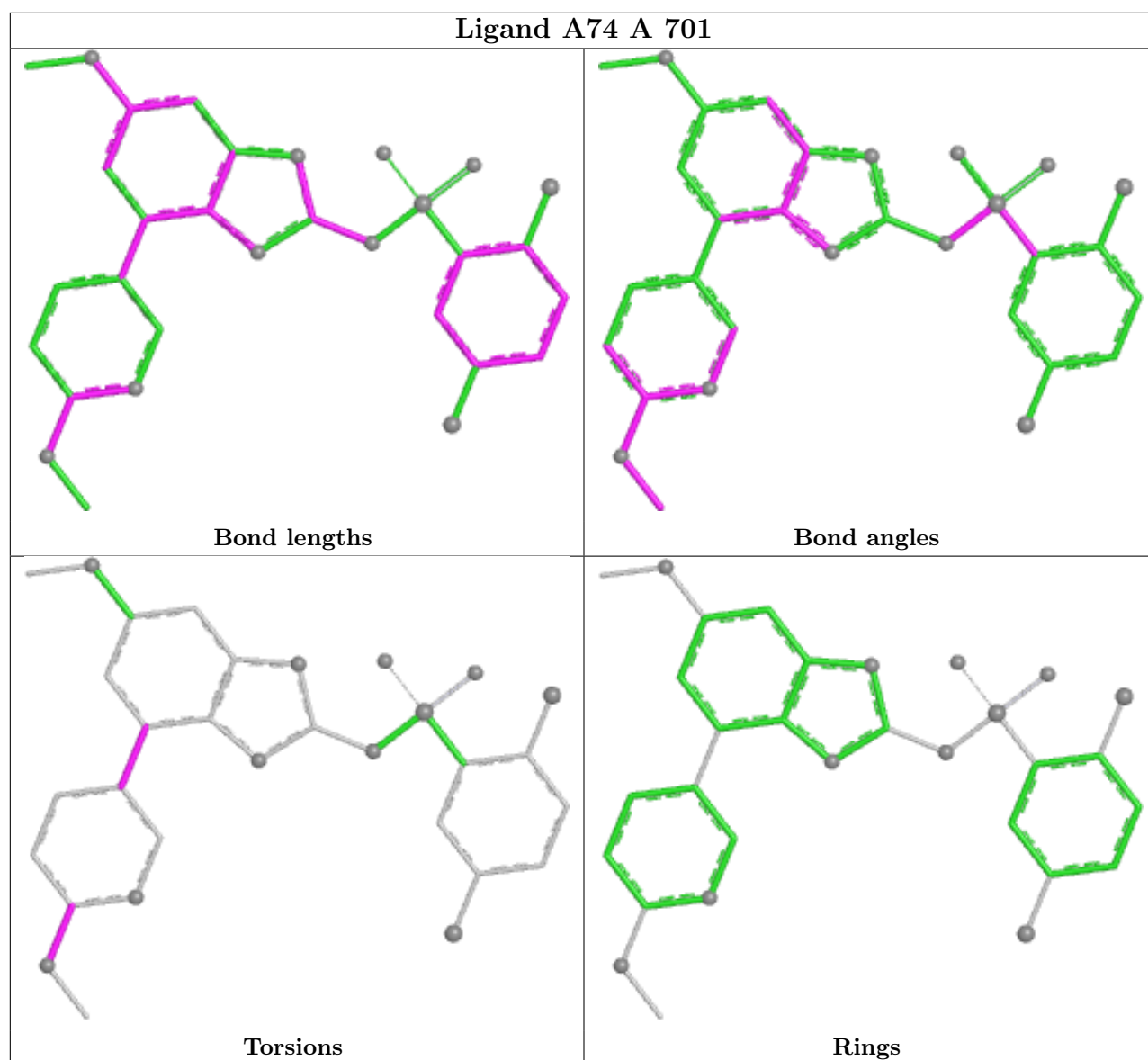
4 monomers are involved in 20 short contacts:

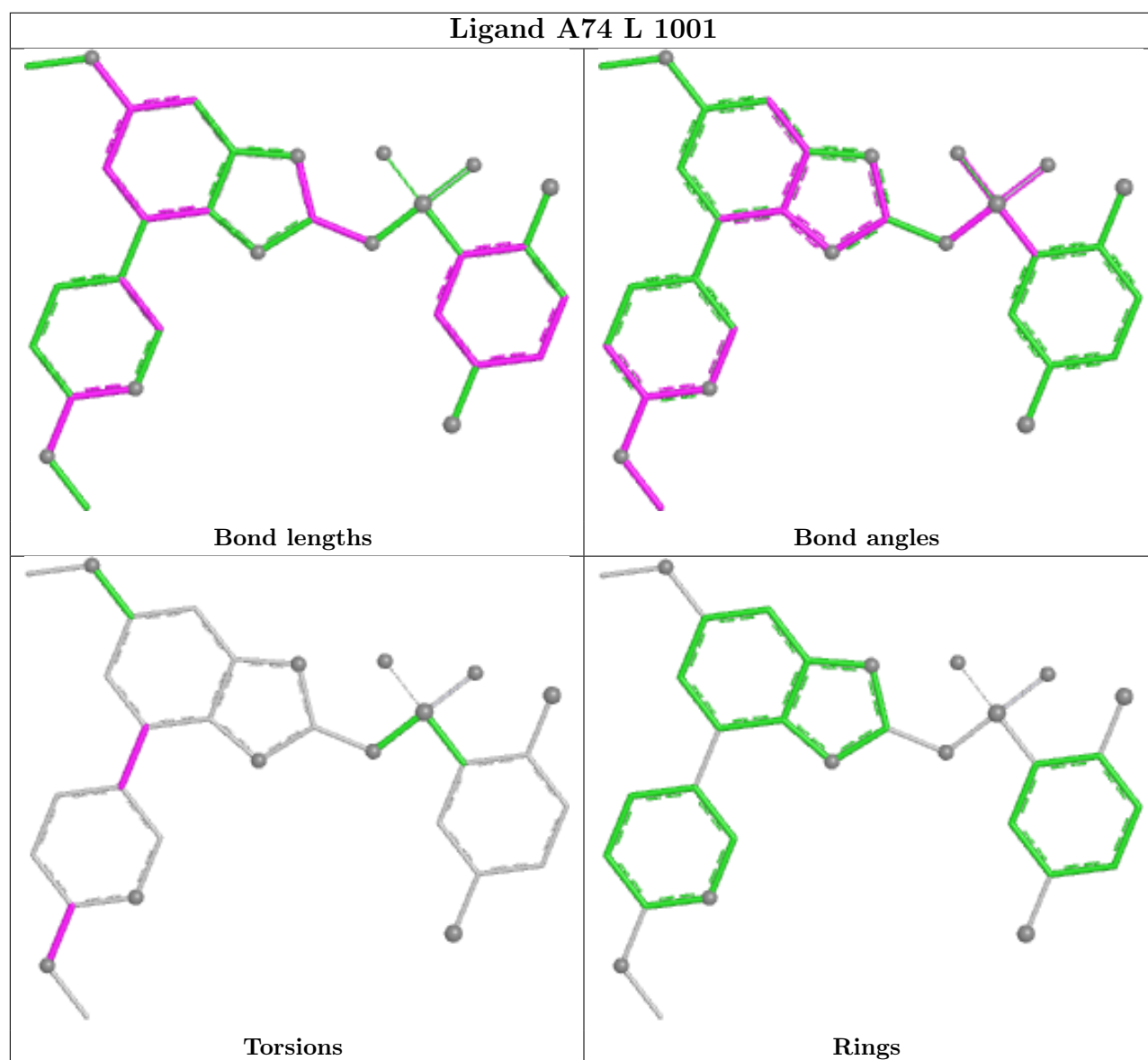
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	A74	4	0
2	A	701	A74	3	0
2	L	1001	A74	7	0
2	H	901	A74	6	0

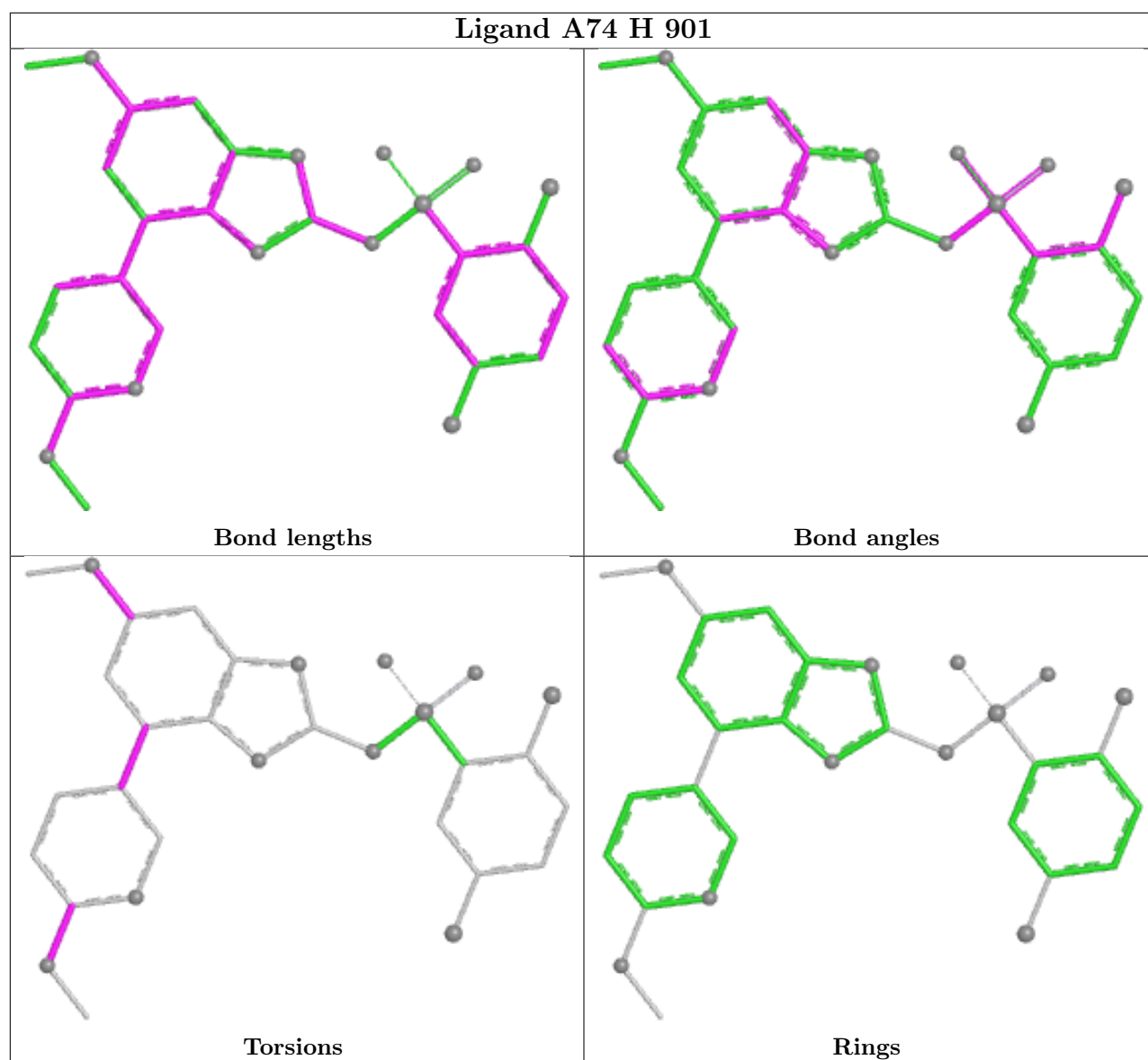
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.