



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:44 AM UTC

PDB ID : 1KKQ / pdb_00001kkq
Title : Crystal structure of the human PPAR-alpha ligand-binding domain in complex with an antagonist GW6471 and a SMRT corepressor motif
Authors : Xu, H.E.; Stanley, T.B.; Montana, V.G.; Lambert, M.H.; Shearer, B.G.; Cobb, J.E.; McKee, D.D.; Galardi, C.M.; Nolte, R.T.; Parks, D.J.
Deposited on : 2001-12-10
Resolution : 3.00 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

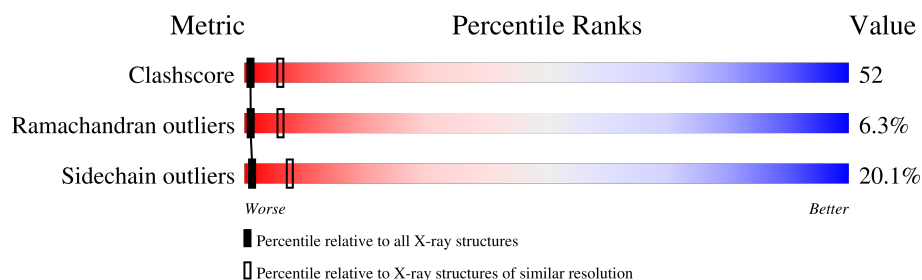
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	269	32% 46% 20% .
1	B	269	37% 45% 15% .
1	C	269	36% 43% 15% 5%
1	D	269	38% 42% 18% .
2	E	19	16% 37% 37% 11%
2	F	19	32% 26% 32% 11%
2	G	19	32% 42% 26%
2	H	19	42% 32% 26%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9606 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.

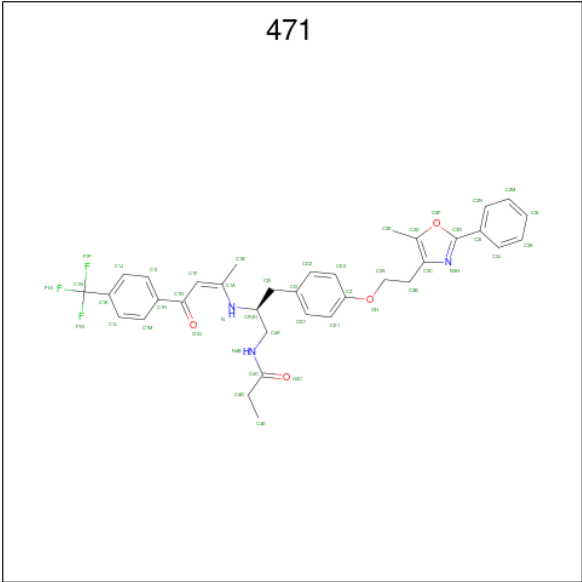
- Molecule 1 is a protein called PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2128	1365	357	388	18			
1	B	269	Total	C	N	O	S	0	0	0
			2128	1365	357	388	18			
1	C	269	Total	C	N	O	S	0	0	0
			2128	1365	357	388	18			
1	D	269	Total	C	N	O	S	0	0	0
			2128	1365	357	388	18			

- Molecule 2 is a protein called NUCLEAR RECEPTOR CO-REPRESSOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	19	Total	C	N	O	S	0	0	0
			145	94	24	25	2			
2	F	19	Total	C	N	O	S	0	0	0
			149	97	25	25	2			
2	G	19	Total	C	N	O	S	0	0	0
			145	94	24	25	2			
2	H	19	Total	C	N	O	S	0	0	0
			145	94	24	25	2			

- Molecule 3 is N-((2S)-2-({(1Z)-1-METHYL-3-OXO-3-[4-(TRIFLUOROMETHYL) PHENYL]PROP-1-ENYL}AMINO)-3-{4-[2-(5-METHYL-2-PHENYL-1,3-OXAZOL-4-YL)ETHOXY]PHENYL}PROPYL)PROPANAMIDE (CCD ID: 471) (formula: C₃₅H₃₆F₃N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			45	35	3	3	4		
3	B	1	Total	C	F	N	O	0	0
			45	35	3	3	4		
3	C	1	Total	C	F	N	O	0	0
			45	35	3	3	4		
3	D	1	Total	C	F	N	O	0	0
			45	35	3	3	4		

- Molecule 4 is water.

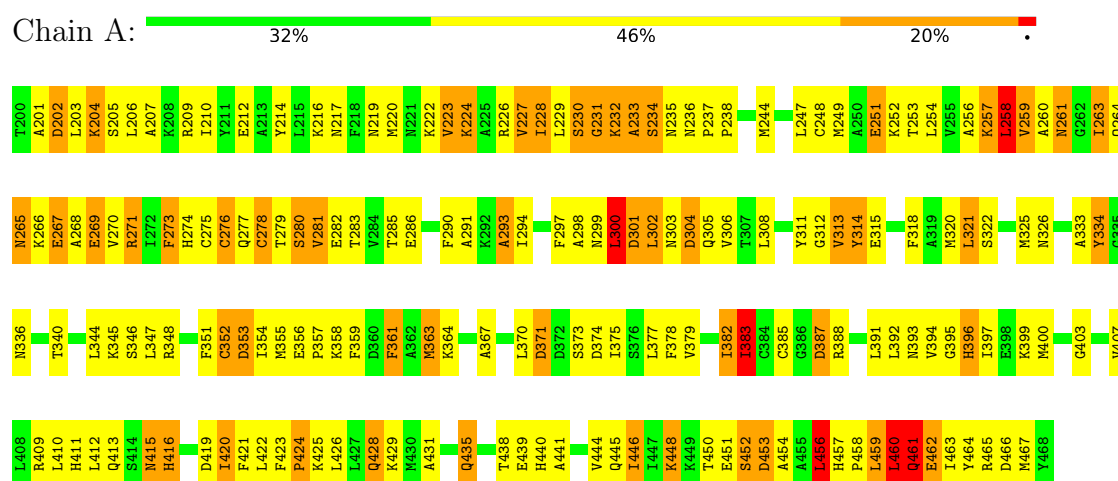
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	108	Total	O	0	0
			108	108		
4	C	55	Total	O	0	0
			55	55		
4	D	87	Total	O	0	0
			87	87		
4	E	4	Total	O	0	0
			4	4		
4	F	10	Total	O	0	0
			10	10		
4	G	1	Total	O	0	0
			1	1		
4	H	4	Total	O	0	0
			4	4		

3 Residue-property plots

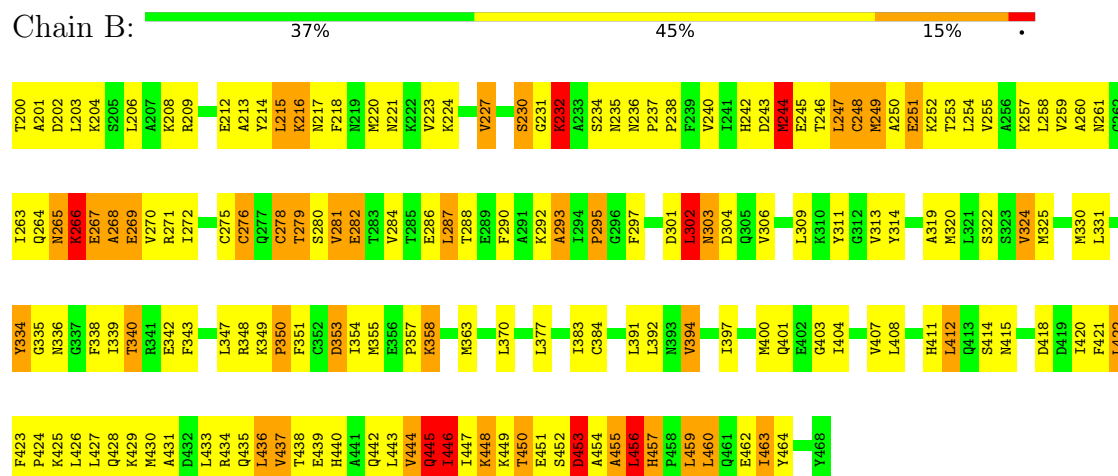
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

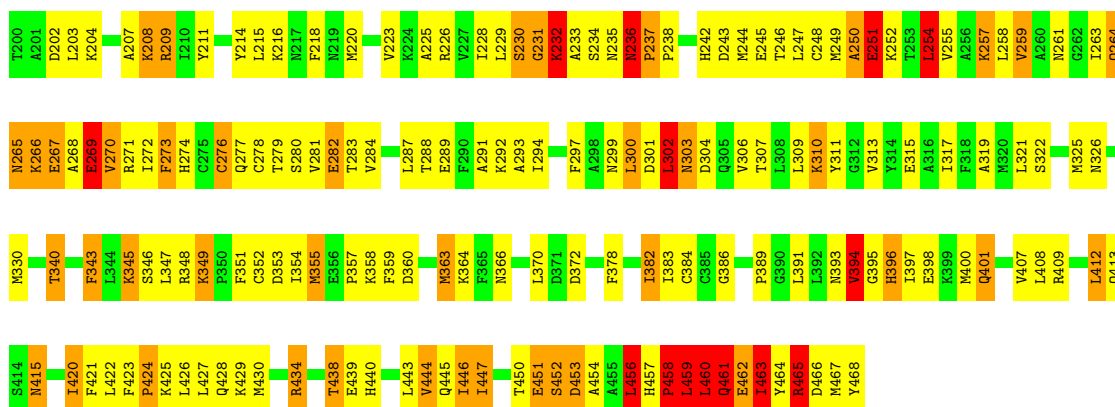


• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR



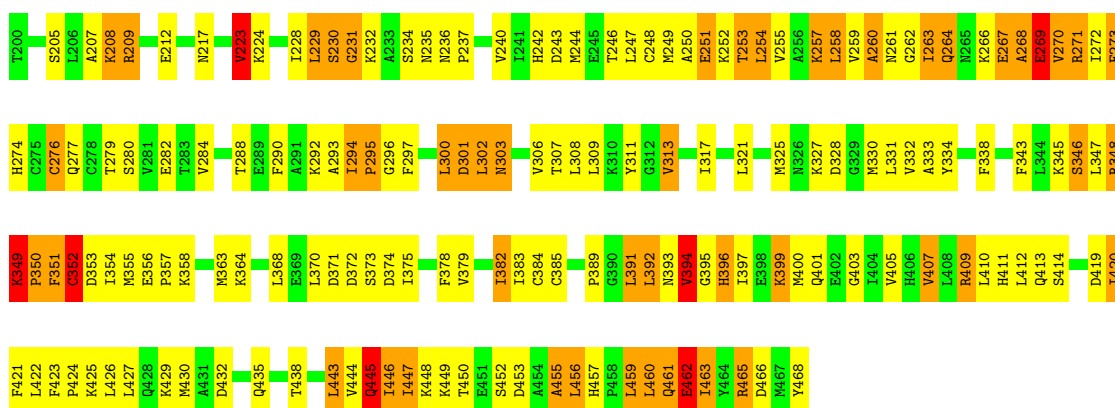
• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR





• Molecule 1: PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR

Chain D: 38% 42% 18%



• Molecule 2: NUCLEAR RECEPTOR CO-REPRESSOR 2

Chain E: 16% 37% 37% 11%



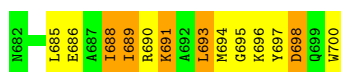
• Molecule 2: NUCLEAR RECEPTOR CO-REPRESSOR 2

Chain F: 32% 26% 32% 11%



• Molecule 2: NUCLEAR RECEPTOR CO-REPRESSOR 2

Chain G: 32% 42% 26%



• Molecule 2: NUCLEAR RECEPTOR CO-REPRESSOR 2



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	103.41 Å 112.77 Å 123.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.99 – 3.00	Depositor
% Data completeness (in resolution range)	98.8 (20.99-3.00)	Depositor
R_{merge}	0.02	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNX 2000	Depositor
R, R_{free}	0.258 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9606	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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:
471

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	0.51	0/2166	1.24	30/2920 (1.0%)
1	B	0.59	0/2166	1.27	30/2920 (1.0%)
1	C	0.50	0/2166	1.27	24/2920 (0.8%)
1	D	0.61	2/2166 (0.1%)	1.17	21/2920 (0.7%)
2	E	0.85	0/147	1.26	3/195 (1.5%)
2	F	0.56	0/151	1.51	4/199 (2.0%)
2	G	0.74	0/147	1.59	3/195 (1.5%)
2	H	0.60	0/147	1.42	2/195 (1.0%)
All	All	0.56	2/9256 (0.0%)	1.25	117/12464 (0.9%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	348	ARG	CA-C	-8.54	1.41	1.52
1	D	348	ARG	C-O	-5.50	1.17	1.24

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	461	GLN	N-CA-C	-18.62	90.69	113.41
1	C	456	LEU	N-CA-C	-12.02	94.32	110.55
1	B	276	CYS	N-CA-C	-11.39	99.74	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	278	CYS	N-CA-C	-11.36	99.39	113.02
2	G	696	LYS	N-CA-C	11.24	127.84	110.42
1	C	276	CYS	N-CA-C	-10.79	99.70	113.72
1	D	302	LEU	N-CA-C	-10.40	100.59	113.18
1	C	266	LYS	N-CA-C	-10.16	93.62	109.07
1	C	451	GLU	N-CA-C	-9.75	90.04	110.80
1	A	446	ILE	N-CA-C	-9.71	100.85	112.98
1	C	444	VAL	N-CA-C	-9.63	104.10	113.53
1	B	267	GLU	N-CA-C	-9.21	91.18	110.80
1	A	282	GLU	N-CA-C	-8.88	101.17	111.03
1	B	230	SER	N-CA-C	-8.85	102.99	113.88
1	A	231	GLY	N-CA-C	8.79	126.31	111.98
1	A	261	ASN	N-CA-C	8.76	120.76	111.03
1	A	278	CYS	N-CA-C	-8.76	103.14	113.21
1	C	203	LEU	N-CA-C	-8.56	102.84	113.20
2	H	692	ALA	N-CA-C	-8.47	102.72	113.23
2	H	697	TYR	N-CA-C	8.36	121.72	107.93
1	A	460	LEU	N-CA-C	-8.30	103.05	113.01
1	B	203	LEU	N-CA-C	-8.26	103.33	113.41
1	D	462	GLU	N-CA-C	8.25	128.38	110.80
1	D	236	ASN	N-CA-C	-8.21	91.66	109.81
1	B	278	CYS	N-CA-C	-8.21	100.22	112.04
1	B	282	GLU	N-CA-C	-8.20	101.06	112.45
2	F	696	LYS	N-CA-C	8.12	121.25	110.53
1	B	453	ASP	CA-C-N	8.06	133.18	122.30
1	B	453	ASP	C-N-CA	8.06	133.18	122.30
2	F	695	GLY	N-CA-C	7.98	132.10	113.18
1	D	270	VAL	N-CA-C	-7.97	104.60	112.17
1	C	270	VAL	N-CA-C	-7.96	103.14	111.58
1	D	450	THR	N-CA-C	-7.96	102.30	110.97
1	B	217	ASN	N-CA-C	7.76	122.75	113.28
1	B	202	ASP	N-CA-C	-7.69	101.56	113.02
1	D	396	HIS	N-CA-C	-7.46	102.30	111.40
1	B	404	ILE	N-CA-C	-7.43	103.62	110.82
1	A	233	ALA	N-CA-C	-7.29	101.14	111.56
1	C	236	ASN	N-CA-C	-7.26	93.76	109.81
2	G	695	GLY	N-CA-C	7.18	130.20	113.18
1	A	249	MET	N-CA-C	-7.17	103.15	110.97
1	D	351	PHE	N-CA-C	7.17	126.06	110.80
1	B	249	MET	N-CA-C	-7.10	103.59	112.90
1	C	237	PRO	N-CA-C	-7.10	102.04	110.70
1	C	458	PRO	N-CA-C	-6.99	98.06	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ALA	N-CA-C	6.93	120.62	111.75
1	B	445	GLN	N-CA-C	-6.92	103.67	111.14
1	D	234	SER	N-CA-C	-6.89	99.74	110.42
1	C	274	HIS	N-CA-C	-6.80	105.53	114.31
1	A	258	LEU	N-CA-C	6.76	118.55	110.44
1	B	414	SER	N-CA-C	6.70	118.58	111.28
1	A	236	ASN	N-CA-C	-6.69	95.02	109.81
1	B	240	VAL	N-CA-C	6.69	118.20	109.58
2	E	692	ALA	N-CA-C	-6.59	105.24	113.28
1	B	293	ALA	N-CA-C	-6.57	105.30	113.38
1	C	459	LEU	N-CA-C	-6.47	105.48	113.19
1	C	465	ARG	N-CA-C	-6.45	100.98	110.52
1	A	453	ASP	N-CA-C	-6.33	104.52	112.93
2	G	694	MET	N-CA-C	6.28	120.95	113.16
1	C	460	LEU	N-CA-C	-5.99	105.80	112.57
1	A	205	SER	N-CA-C	-5.99	105.96	113.20
1	C	453	ASP	N-CA-C	-5.99	98.05	110.80
1	A	416	HIS	CA-C-N	5.98	127.31	119.84
1	A	416	HIS	C-N-CA	5.98	127.31	119.84
1	A	257	LYS	N-CA-C	-5.97	103.52	112.54
1	D	294	ILE	CA-C-N	5.97	127.31	119.84
1	D	294	ILE	C-N-CA	5.97	127.31	119.84
2	E	685	LEU	N-CA-C	-5.97	104.12	113.02
1	A	293	ALA	N-CA-C	-5.96	104.67	113.61
1	D	261	ASN	N-CA-C	5.94	120.14	113.01
1	D	217	ASN	N-CA-C	5.88	120.74	113.50
1	A	462	GLU	N-CA-C	-5.86	98.31	110.80
1	D	240	VAL	N-CA-C	5.86	116.74	108.36
1	B	223	VAL	N-CA-C	-5.85	104.92	110.42
1	D	374	ASP	N-CA-C	-5.81	104.37	112.45
2	F	692	ALA	N-CA-C	-5.76	104.97	112.23
1	A	383	ILE	N-CA-C	-5.76	105.23	110.82
1	A	228	ILE	N-CA-C	-5.75	105.12	110.53
1	D	328	ASP	N-CA-C	5.71	120.41	113.38
1	B	290	PHE	N-CA-C	-5.67	105.00	111.07
1	B	453	ASP	N-CA-C	-5.66	98.73	110.80
1	A	314	TYR	N-CA-C	5.60	117.46	111.36
1	A	281	VAL	N-CA-C	-5.59	97.71	109.34
1	B	266	LYS	CB-CA-C	5.58	119.64	110.88
1	C	452	SER	N-CA-C	-5.52	99.03	110.80
1	B	311	TYR	N-CA-C	5.50	119.25	112.54
1	A	440	HIS	N-CA-C	-5.43	105.05	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	PRO	N-CA-C	-5.42	106.47	113.57
1	B	340	THR	N-CA-C	5.41	118.16	110.10
1	C	273	PHE	N-CA-C	-5.33	106.27	114.16
1	C	355	MET	N-CA-C	5.33	118.00	111.82
1	A	224	LYS	N-CA-C	-5.33	105.37	111.07
1	D	419	ASP	N-CA-C	-5.31	97.99	107.28
1	B	457	HIS	CA-C-N	-5.29	113.22	119.84
1	B	457	HIS	C-N-CA	-5.29	113.22	119.84
1	A	313	VAL	N-CA-C	5.28	115.90	110.36
1	D	273	PHE	N-CA-C	-5.27	105.13	112.45
2	F	697	TYR	N-CA-C	5.26	116.00	107.32
1	D	368	LEU	N-CA-C	-5.23	106.85	113.18
2	E	683	MET	N-CA-C	-5.22	99.67	110.80
1	A	203	LEU	N-CA-C	-5.21	106.69	113.16
1	A	267	GLU	N-CA-C	-5.21	103.06	110.35
1	A	456	LEU	N-CA-C	-5.21	103.44	110.68
1	D	396	HIS	CB-CA-C	-5.20	102.06	110.79
1	B	265	ASN	CB-CA-C	-5.20	99.04	110.99
1	A	461	GLN	CB-CA-C	-5.19	102.47	110.78
1	C	415	ASN	N-CA-C	-5.13	107.19	113.50
1	D	460	LEU	N-CA-C	-5.12	106.23	113.20
1	B	456	LEU	CA-C-N	-5.10	114.01	123.55
1	B	456	LEU	C-N-CA	-5.10	114.01	123.55
1	A	451	GLU	CB-CA-C	5.05	118.88	110.90
1	C	424	PRO	N-CA-C	-5.05	107.82	114.03
1	D	427	LEU	N-CA-C	-5.05	105.78	111.28
1	C	319	ALA	N-CA-C	-5.04	104.74	111.24
1	B	266	LYS	N-CA-C	5.03	116.45	111.07
1	B	281	VAL	N-CA-C	-5.01	107.97	113.43
1	C	434	ARG	N-CA-C	-5.00	106.69	112.89

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	349	LYS	Mainchain

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	2128	0	2168	213	0
1	B	2128	0	2168	217	0
1	C	2128	0	2168	239	0
1	D	2128	0	2168	220	0
2	E	145	0	138	36	0
2	F	149	0	149	39	0
2	G	145	0	138	29	0
2	H	145	0	138	18	0
3	A	45	0	36	1	0
3	B	45	0	35	8	0
3	C	45	0	36	2	0
3	D	45	0	35	3	0
4	A	61	0	0	3	0
4	B	108	0	0	5	0
4	C	55	0	0	6	0
4	D	87	0	0	8	0
4	E	4	0	0	1	0
4	F	10	0	0	3	0
4	G	1	0	0	1	0
4	H	4	0	0	1	0
All	All	9606	0	9377	972	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 52.

All (972) 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)
2:G:688:ILE:HD13	2:G:689:ILE:N	1.32	1.43
1:D:348:ARG:O	1:D:349:LYS:CG	1.74	1.35
2:G:685:LEU:O	2:G:688:ILE:CD1	1.92	1.16
1:A:269:GLU:HG3	1:A:348:ARG:HH11	1.09	1.16
1:D:348:ARG:O	1:D:349:LYS:HG2	1.33	1.14
2:E:685:LEU:HD23	2:E:685:LEU:H	1.12	1.14
1:A:207:ALA:HB2	1:A:407:VAL:HG11	1.29	1.14
1:A:258:LEU:HD22	1:A:263:ILE:HG13	1.30	1.13
1:A:269:GLU:HG3	1:A:348:ARG:NH1	1.64	1.12
2:G:688:ILE:CD1	2:G:689:ILE:H	1.64	1.10
1:B:200:THR:O	1:B:204:LYS:HD3	1.48	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:LEU:HD22	1:C:263:ILE:HD12	1.31	1.09
1:A:227:VAL:O	1:A:231:GLY:HA3	1.53	1.09
1:D:348:ARG:O	1:D:349:LYS:CB	1.99	1.08
2:E:685:LEU:HD23	2:E:685:LEU:N	1.67	1.08
1:D:457:HIS:HD2	1:D:459:LEU:HB2	1.15	1.05
1:D:457:HIS:CD2	1:D:459:LEU:HB2	1.91	1.05
1:C:231:GLY:O	1:C:233:ALA:N	1.90	1.05
1:A:456:LEU:HD22	1:A:456:LEU:H	1.21	1.03
2:E:683:MET:HE3	2:E:683:MET:HA	1.40	1.03
1:B:456:LEU:HD23	1:B:456:LEU:H	1.23	1.02
1:B:456:LEU:HD23	1:B:456:LEU:N	1.74	1.02
1:B:459:LEU:HD12	1:B:459:LEU:O	1.58	1.02
1:C:300:LEU:HD12	1:C:300:LEU:H	1.22	1.01
1:D:209:ARG:HD2	2:H:700:TRP:HZ3	1.23	1.01
2:G:685:LEU:O	2:G:688:ILE:HD12	1.58	1.00
1:D:268:ALA:HB2	1:D:271:ARG:HH21	1.27	0.99
1:D:244:MET:HE1	1:D:268:ALA:HB3	1.42	0.98
2:G:685:LEU:O	2:G:688:ILE:HD11	1.63	0.97
2:G:688:ILE:CD1	2:G:689:ILE:N	2.23	0.96
1:A:461:GLN:HG3	1:A:464:TYR:CD2	2.01	0.95
1:A:420:ILE:HD13	1:A:421:PHE:H	1.31	0.95
2:G:688:ILE:HD13	2:G:689:ILE:H	0.88	0.95
1:B:445:GLN:HE21	1:B:445:GLN:HA	1.31	0.94
1:C:230:SER:HB2	4:C:783:HOH:O	1.66	0.94
1:A:257:LYS:C	1:A:258:LEU:HD23	1.92	0.93
1:D:272:ILE:O	1:D:276:CYS:HB2	1.68	0.92
1:C:420:ILE:HD13	1:C:421:PHE:N	1.84	0.92
2:G:688:ILE:HD12	2:G:688:ILE:H	1.32	0.91
1:A:363:MET:HE3	1:A:363:MET:HA	1.52	0.91
1:C:237:PRO:HB2	1:C:238:PRO:HD2	1.53	0.91
1:D:268:ALA:CB	1:D:271:ARG:HH21	1.83	0.91
1:D:268:ALA:HB2	1:D:271:ARG:NH2	1.87	0.90
1:D:391:LEU:HD12	1:D:397:ILE:HD12	1.53	0.90
1:C:209:ARG:HH22	1:C:293:ALA:HB1	1.35	0.90
1:B:460:LEU:N	1:B:460:LEU:HD23	1.85	0.90
1:C:317:ILE:O	1:C:321:LEU:HB2	1.73	0.89
2:G:688:ILE:HD12	2:G:688:ILE:N	1.87	0.89
1:B:450:THR:HG22	1:B:451:GLU:HG3	1.53	0.89
1:D:460:LEU:HD12	1:D:460:LEU:H	1.38	0.89
1:A:273:PHE:HD2	1:A:273:PHE:O	1.55	0.88
1:A:273:PHE:O	1:A:273:PHE:CD2	2.27	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:LEU:HD13	1:C:456:LEU:N	1.88	0.88
2:E:685:LEU:HA	4:E:169:HOH:O	1.70	0.88
1:C:230:SER:O	1:C:232:LYS:N	2.07	0.88
1:B:449:LYS:HA	1:B:452:SER:OG	1.73	0.88
1:B:451:GLU:O	1:B:453:ASP:OD1	1.92	0.88
1:B:230:SER:O	1:B:232:LYS:HG3	1.73	0.88
1:C:461:GLN:O	1:C:465:ARG:HD2	1.72	0.87
1:D:230:SER:O	1:D:232:LYS:HD2	1.75	0.87
1:C:386:GLY:HA3	1:C:398:GLU:HG3	1.57	0.87
1:B:201:ALA:HA	1:B:204:LYS:HE2	1.56	0.86
1:D:459:LEU:O	1:D:459:LEU:HD12	1.75	0.85
1:A:207:ALA:HB2	1:A:407:VAL:CG1	2.06	0.85
1:A:223:VAL:O	1:A:227:VAL:HG23	1.76	0.85
1:A:258:LEU:HD22	1:A:263:ILE:CG1	2.06	0.85
1:C:457:HIS:CD2	1:C:458:PRO:HD3	2.12	0.84
1:A:456:LEU:HD22	1:A:456:LEU:N	1.93	0.84
1:D:457:HIS:HD2	1:D:459:LEU:CB	1.90	0.84
1:A:219:ASN:O	1:A:224:LYS:NZ	2.10	0.84
1:B:384:CYS:O	1:B:401:GLN:HB2	1.77	0.84
1:A:457:HIS:CG	1:A:458:PRO:HD2	2.12	0.84
1:A:461:GLN:HA	1:A:464:TYR:HB3	1.59	0.83
1:C:300:LEU:HD12	1:C:300:LEU:N	1.91	0.83
2:E:685:LEU:N	2:E:685:LEU:CD2	2.39	0.83
1:A:412:LEU:HD11	1:A:426:LEU:HD12	1.59	0.83
1:D:255:VAL:H	1:D:258:LEU:HD11	1.43	0.83
1:A:244:MET:HE1	1:A:268:ALA:HB2	1.60	0.83
1:A:420:ILE:HD13	1:A:421:PHE:N	1.92	0.83
1:C:409:ARG:O	1:C:413:GLN:HB2	1.78	0.83
1:B:355:MET:HE1	3:B:776:471:HCE1	1.61	0.83
1:B:457:HIS:C	1:B:459:LEU:H	1.87	0.82
1:D:255:VAL:HB	1:D:258:LEU:HG	1.61	0.82
1:B:272:ILE:O	1:B:276:CYS:HB2	1.79	0.82
2:G:688:ILE:CD1	2:G:689:ILE:HG23	2.10	0.82
1:A:257:LYS:HE2	1:A:261:ASN:ND2	1.95	0.82
1:D:378:PHE:O	1:D:382:ILE:HG23	1.80	0.82
1:C:360:ASP:OD2	1:C:364:LYS:HE3	1.80	0.81
1:A:456:LEU:H	1:A:456:LEU:CD2	1.92	0.81
1:A:285:THR:HG23	2:E:692:ALA:HB1	1.63	0.81
1:B:457:HIS:ND1	1:B:459:LEU:HB2	1.95	0.81
2:E:697:TYR:O	2:E:698:ASP:HB2	1.80	0.81
1:D:209:ARG:CD	2:H:700:TRP:HZ3	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:ASN:OD1	1:C:236:ASN:O	1.99	0.80
1:C:315:GLU:HB2	1:C:382:ILE:HD13	1.64	0.80
1:D:244:MET:CE	1:D:268:ALA:HB3	2.10	0.80
2:H:697:TYR:O	2:H:698:ASP:HB2	1.81	0.80
1:A:396:HIS:O	1:A:399:LYS:HG2	1.82	0.80
1:C:209:ARG:NH2	1:C:293:ALA:HB1	1.96	0.80
1:A:277:GLN:C	1:A:279:THR:H	1.89	0.79
2:F:696:LYS:HD2	2:F:696:LYS:O	1.82	0.79
1:A:374:ASP:OD2	1:A:416:HIS:HE1	1.65	0.79
1:A:273:PHE:CZ	1:A:454:ALA:O	2.36	0.79
1:B:459:LEU:O	1:B:459:LEU:CD1	2.31	0.78
2:E:697:TYR:O	2:E:697:TYR:HD1	1.66	0.78
2:G:688:ILE:HD11	2:G:689:ILE:HG23	1.65	0.78
1:C:235:ASN:OD1	1:C:236:ASN:N	2.16	0.78
1:B:444:VAL:HA	1:B:447:ILE:HD12	1.66	0.78
2:F:696:LYS:HD2	2:F:696:LYS:C	2.08	0.77
1:C:232:LYS:O	1:C:232:LYS:HG2	1.84	0.77
1:C:459:LEU:O	1:C:459:LEU:HG	1.82	0.77
1:C:248:CYS:SG	1:C:271:ARG:NH2	2.58	0.77
1:B:412:LEU:HD21	1:B:426:LEU:HD12	1.67	0.77
1:C:258:LEU:CD2	1:C:263:ILE:HD12	2.12	0.77
1:B:201:ALA:O	1:B:204:LYS:HE2	1.85	0.76
1:D:230:SER:O	1:D:232:LYS:CD	2.33	0.76
2:E:683:MET:HG3	2:E:684:GLY:H	1.50	0.76
1:A:263:ILE:HA	1:A:266:LYS:HZ3	1.50	0.76
1:C:363:MET:HE3	1:C:363:MET:HA	1.68	0.76
1:B:454:ALA:O	1:B:455:ALA:HB2	1.84	0.76
1:A:321:LEU:O	1:A:325:MET:HG3	1.86	0.76
1:D:391:LEU:CD1	1:D:397:ILE:HD12	2.15	0.76
2:G:688:ILE:HD13	2:G:688:ILE:C	2.08	0.76
1:A:269:GLU:CG	1:A:348:ARG:HH11	1.95	0.75
1:D:345:LYS:O	1:D:352:CYS:HB3	1.85	0.75
1:D:394:VAL:HG13	1:D:394:VAL:O	1.86	0.75
1:D:255:VAL:HB	1:D:258:LEU:CG	2.15	0.75
1:A:248:CYS:SG	1:A:271:ARG:NH2	2.59	0.75
1:A:396:HIS:HB3	1:A:399:LYS:NZ	2.01	0.75
1:C:297:PHE:HA	1:C:300:LEU:HD11	1.67	0.75
1:A:251:GLU:OE1	1:A:271:ARG:HG2	1.87	0.75
1:C:461:GLN:NE2	1:C:461:GLN:C	2.45	0.75
2:H:689:ILE:O	2:H:693:LEU:HD22	1.86	0.75
1:D:251:GLU:HA	1:D:254:LEU:HB2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ALA:C	1:A:334:TYR:HD2	1.94	0.75
1:D:274:HIS:O	1:D:277:GLN:HB2	1.87	0.75
1:D:302:LEU:HD13	1:D:302:LEU:O	1.87	0.74
1:D:348:ARG:C	1:D:349:LYS:HG2	2.11	0.74
1:A:311:TYR:HB2	1:A:388:ARG:HD2	1.69	0.74
1:C:453:ASP:CG	1:C:454:ALA:H	1.95	0.74
1:B:355:MET:CE	3:B:776:471:HCE1	2.18	0.74
1:B:348:ARG:NH2	1:B:351:PHE:HE2	1.85	0.73
1:B:201:ALA:HA	1:B:204:LYS:CE	2.18	0.73
1:D:209:ARG:HD2	2:H:700:TRP:CZ3	2.16	0.73
1:C:461:GLN:C	1:C:461:GLN:HE21	1.96	0.73
1:A:257:LYS:O	1:A:257:LYS:HG2	1.87	0.73
1:A:409:ARG:HG2	1:A:413:GLN:HE21	1.52	0.73
1:A:467:MET:HE3	1:A:467:MET:HA	1.70	0.73
1:C:292:LYS:HD3	2:G:693:LEU:HD12	1.71	0.73
2:F:685:LEU:HA	4:F:240:HOH:O	1.87	0.73
1:C:420:ILE:HD13	1:C:421:PHE:H	1.53	0.73
1:C:223:VAL:HG23	1:C:372:ASP:OD2	1.89	0.72
1:C:251:GLU:HA	1:C:254:LEU:HB2	1.70	0.72
1:D:232:LYS:HE2	4:D:828:HOH:O	1.88	0.72
1:D:249:MET:O	1:D:253:THR:HG23	1.89	0.72
1:A:456:LEU:HD11	3:A:775:471:H4E1	1.71	0.72
1:D:348:ARG:O	1:D:349:LYS:HB2	1.89	0.72
2:G:688:ILE:CD1	2:G:689:ILE:CG2	2.68	0.72
1:B:270:VAL:HG13	1:B:454:ALA:CB	2.20	0.72
1:A:306:VAL:HG13	2:E:689:ILE:HD11	1.71	0.72
1:B:314:TYR:HE1	3:B:776:471:H4A2	1.53	0.72
1:B:334:TYR:N	1:B:334:TYR:CD1	2.57	0.72
1:C:279:THR:HG21	4:C:816:HOH:O	1.90	0.72
1:B:227:VAL:HA	1:B:231:GLY:HA3	1.72	0.72
1:A:334:TYR:N	1:A:334:TYR:CD2	2.56	0.72
1:C:313:VAL:O	1:C:317:ILE:HG13	1.89	0.72
1:D:457:HIS:O	1:D:460:LEU:HD12	1.89	0.72
1:D:349:LYS:HD3	1:D:352:CYS:SG	2.30	0.71
1:B:230:SER:O	1:B:232:LYS:HE2	1.89	0.71
1:B:292:LYS:HZ1	2:F:696:LYS:CE	2.02	0.71
1:B:391:LEU:HD13	1:B:397:ILE:HD12	1.71	0.71
1:A:248:CYS:O	1:A:252:LYS:HB2	1.90	0.71
1:D:420:ILE:HD11	1:D:421:PHE:CE1	2.25	0.71
1:B:258:LEU:HD21	1:B:263:ILE:HD12	1.71	0.71
1:D:448:LYS:O	1:D:452:SER:HA	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:VAL:HA	2:F:689:ILE:HD11	1.72	0.71
1:C:465:ARG:O	1:C:465:ARG:HD3	1.91	0.71
1:B:270:VAL:CG1	1:B:454:ALA:CB	2.68	0.71
1:C:257:LYS:O	1:C:257:LYS:HG2	1.90	0.71
2:E:682:ASN:O	2:E:683:MET:HB2	1.90	0.71
1:C:244:MET:HE3	1:C:268:ALA:HB3	1.70	0.71
1:D:396:HIS:HB3	4:D:838:HOH:O	1.91	0.71
1:D:449:LYS:HA	1:D:452:SER:OG	1.91	0.71
1:A:300:LEU:HD11	1:A:400:MET:HE1	1.71	0.70
1:C:446:ILE:O	1:C:446:ILE:HG22	1.89	0.70
1:D:412:LEU:HD11	1:D:426:LEU:HD12	1.71	0.70
1:A:263:ILE:HA	1:A:266:LYS:NZ	2.06	0.70
1:B:247:LEU:O	1:B:247:LEU:HD12	1.89	0.70
1:D:348:ARG:HG3	1:D:349:LYS:N	2.03	0.70
1:D:409:ARG:HG2	1:D:410:LEU:HD23	1.73	0.70
1:B:235:ASN:O	1:B:236:ASN:HB3	1.91	0.70
1:C:378:PHE:O	1:C:382:ILE:HG23	1.91	0.70
1:C:460:LEU:HD23	1:C:464:TYR:CE2	2.27	0.70
1:B:265:ASN:CG	1:B:265:ASN:O	2.27	0.70
1:D:235:ASN:C	1:D:235:ASN:ND2	2.48	0.70
1:B:292:LYS:HE3	2:F:696:LYS:HE2	1.73	0.69
1:D:297:PHE:HA	1:D:300:LEU:HD11	1.74	0.69
2:G:688:ILE:CD1	2:G:688:ILE:N	2.54	0.69
2:H:683:MET:HG3	2:H:684:GLY:H	1.58	0.69
1:A:274:HIS:HA	1:A:277:GLN:HE21	1.58	0.69
1:A:457:HIS:HB3	1:A:459:LEU:HD22	1.74	0.69
2:G:686:GLU:OE2	2:G:690:ARG:NH1	2.26	0.69
1:A:244:MET:HE1	1:A:271:ARG:HH21	1.57	0.69
1:B:334:TYR:N	1:B:334:TYR:HD1	1.91	0.69
1:C:266:LYS:O	1:C:267:GLU:C	2.35	0.69
1:D:457:HIS:C	1:D:459:LEU:H	2.01	0.69
1:B:446:ILE:O	1:B:446:ILE:HG23	1.92	0.68
1:C:309:LEU:O	1:C:313:VAL:HB	1.92	0.68
1:D:351:PHE:O	1:D:353:ASP:N	2.26	0.68
2:G:685:LEU:HA	4:G:260:HOH:O	1.93	0.68
1:A:258:LEU:CD2	1:A:263:ILE:HG13	2.17	0.68
1:C:273:PHE:O	1:C:277:GLN:HG3	1.94	0.68
1:D:242:HIS:CE1	1:D:243:ASP:OD2	2.46	0.68
1:C:450:THR:O	1:C:451:GLU:HG2	1.94	0.68
1:A:266:LYS:O	1:A:267:GLU:C	2.37	0.68
1:B:201:ALA:CA	1:B:204:LYS:HE2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ASN:HB3	1:A:396:HIS:CE1	2.28	0.68
1:D:300:LEU:HD12	1:D:300:LEU:H	1.59	0.68
1:A:315:GLU:HB2	1:A:382:ILE:HD13	1.75	0.67
1:D:423:PHE:HB3	1:D:424:PRO:HD3	1.75	0.67
2:F:694:MET:HE2	2:F:694:MET:N	2.09	0.67
1:A:227:VAL:O	1:A:231:GLY:CA	2.39	0.67
1:D:447:ILE:HD12	1:D:447:ILE:N	2.09	0.67
2:G:688:ILE:HD11	2:G:689:ILE:CG2	2.24	0.67
1:B:450:THR:CG2	1:B:451:GLU:HG3	2.24	0.67
1:A:258:LEU:HB3	1:A:263:ILE:HG12	1.76	0.67
1:C:272:ILE:O	1:C:272:ILE:HG22	1.94	0.67
1:A:361:PHE:CD1	1:A:361:PHE:C	2.72	0.67
1:D:300:LEU:HD12	1:D:300:LEU:N	2.10	0.67
1:D:465:ARG:HG2	1:D:466:ASP:OD1	1.94	0.67
1:D:465:ARG:HG3	1:D:465:ARG:HH11	1.60	0.67
1:A:387:ASP:OD2	1:A:387:ASP:N	2.27	0.67
1:C:461:GLN:O	1:C:461:GLN:NE2	2.28	0.67
1:B:319:ALA:HB2	1:B:433:LEU:HD11	1.77	0.67
1:B:348:ARG:HH22	1:B:351:PHE:HE2	1.43	0.67
1:A:263:ILE:HD13	1:A:263:ILE:H	1.58	0.66
1:C:456:LEU:N	1:C:456:LEU:CD1	2.58	0.66
1:B:325:MET:HG2	1:B:330:MET:HB3	1.76	0.66
1:B:267:GLU:OE1	1:B:348:ARG:NH2	2.28	0.66
1:C:235:ASN:CG	1:C:236:ASN:H	2.03	0.66
1:B:275:CYS:HA	1:B:278:CYS:SG	2.34	0.66
1:D:382:ILE:HD12	1:D:382:ILE:O	1.95	0.66
1:D:345:LYS:HA	1:D:352:CYS:HA	1.77	0.66
1:B:270:VAL:HG13	1:B:454:ALA:HB3	1.78	0.66
2:G:697:TYR:O	2:G:698:ASP:HB2	1.95	0.66
1:B:453:ASP:OD1	1:B:453:ASP:N	2.27	0.66
1:A:461:GLN:HG3	1:A:464:TYR:HD2	1.61	0.65
1:A:259:VAL:O	1:A:259:VAL:CG1	2.44	0.65
1:A:419:ASP:HB3	1:A:422:LEU:HB2	1.78	0.65
1:C:232:LYS:O	1:C:232:LYS:CG	2.43	0.65
1:A:411:HIS:O	1:A:415:ASN:HB2	1.97	0.65
1:A:457:HIS:CD2	1:A:458:PRO:HD2	2.31	0.65
1:B:309:LEU:O	1:B:313:VAL:HB	1.97	0.65
1:D:422:LEU:HB3	4:D:795:HOH:O	1.96	0.65
1:D:263:ILE:HA	1:D:266:LYS:HE3	1.78	0.65
1:A:399:LYS:HG3	1:A:400:MET:N	2.11	0.65
1:A:428:GLN:O	1:A:431:ALA:HB3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ASN:O	1:C:395:GLY:N	2.29	0.65
1:A:285:THR:HG23	2:E:692:ALA:CB	2.26	0.65
1:B:243:ASP:OD1	1:B:245:GLU:HB3	1.96	0.65
1:D:348:ARG:CG	1:D:349:LYS:N	2.59	0.65
1:B:354:ILE:O	1:B:357:PRO:HD2	1.98	0.64
1:C:438:THR:HG22	1:C:439:GLU:N	2.11	0.64
1:D:348:ARG:C	1:D:349:LYS:CG	2.66	0.64
1:A:391:LEU:HD13	1:A:397:ILE:HD12	1.79	0.64
1:A:300:LEU:HD21	1:A:400:MET:CE	2.28	0.64
1:A:403:GLY:O	1:A:407:VAL:HG23	1.98	0.64
1:B:440:HIS:O	1:B:444:VAL:HB	1.98	0.64
1:D:409:ARG:HG2	1:D:410:LEU:N	2.11	0.64
1:D:244:MET:HE1	1:D:268:ALA:CB	2.21	0.64
1:D:446:ILE:C	1:D:447:ILE:HD12	2.22	0.64
1:B:331:LEU:HD22	1:B:335:GLY:HA2	1.80	0.64
1:A:420:ILE:HD11	1:A:421:PHE:CD1	2.33	0.64
1:B:455:ALA:O	1:B:457:HIS:N	2.31	0.64
1:C:235:ASN:CG	1:C:236:ASN:N	2.55	0.64
1:C:456:LEU:HD13	1:C:456:LEU:H	1.61	0.64
1:C:461:GLN:HE22	1:C:465:ARG:NH1	1.96	0.64
1:B:218:PHE:CE1	1:B:320:MET:HE1	2.32	0.64
1:B:456:LEU:N	1:B:456:LEU:CD2	2.48	0.64
2:E:683:MET:HA	2:E:683:MET:CE	2.21	0.64
1:B:445:GLN:C	1:B:447:ILE:H	2.05	0.63
1:C:463:ILE:O	1:C:464:TYR:CD2	2.52	0.63
2:G:688:ILE:HD13	2:G:689:ILE:CG2	2.28	0.63
1:C:450:THR:O	1:C:450:THR:HG22	1.97	0.63
1:D:445:GLN:HE21	1:D:445:GLN:HA	1.63	0.63
1:B:358:LYS:HE3	1:B:436:LEU:HD21	1.80	0.63
1:B:279:THR:HG21	4:B:794:HOH:O	1.98	0.63
1:A:301:ASP:C	1:A:301:ASP:OD1	2.42	0.63
1:D:309:LEU:HB3	2:H:689:ILE:HD12	1.81	0.63
1:C:396:HIS:ND1	1:C:396:HIS:N	2.47	0.62
1:B:237:PRO:HB2	1:B:238:PRO:HD2	1.81	0.62
1:A:435:GLN:O	1:A:435:GLN:HG3	1.97	0.62
1:D:273:PHE:O	1:D:277:GLN:HG2	1.98	0.62
2:F:697:TYR:CG	2:F:697:TYR:O	2.51	0.62
1:C:268:ALA:HA	1:C:271:ARG:HD3	1.80	0.62
1:A:333:ALA:C	1:A:334:TYR:CD2	2.78	0.62
1:A:345:LYS:HG3	1:A:345:LYS:O	1.99	0.62
1:A:216:LYS:O	1:A:216:LYS:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:PHE:HB3	1:A:424:PRO:HD3	1.82	0.62
1:D:297:PHE:O	1:D:300:LEU:CD1	2.47	0.62
1:D:348:ARG:O	1:D:349:LYS:HG3	1.93	0.62
1:A:263:ILE:CG2	1:A:266:LYS:HZ3	2.13	0.62
1:A:298:ALA:HA	1:A:305:GLN:HE22	1.64	0.62
1:C:251:GLU:HA	1:C:254:LEU:HD22	1.81	0.62
1:C:457:HIS:CG	1:C:458:PRO:CD	2.83	0.62
1:B:248:CYS:O	1:B:252:LYS:HB2	1.99	0.62
1:B:270:VAL:HG21	1:B:453:ASP:OD2	1.99	0.62
1:A:233:ALA:O	1:A:234:SER:HB2	1.97	0.62
1:C:297:PHE:O	1:C:300:LEU:HD13	1.98	0.62
1:D:399:LYS:O	1:D:399:LYS:HG3	1.97	0.62
1:D:270:VAL:CG2	1:D:348:ARG:NH2	2.64	0.61
1:D:373:SER:OG	1:D:411:HIS:CE1	2.53	0.61
1:A:378:PHE:O	1:A:382:ILE:HG23	2.01	0.61
1:D:325:MET:HG2	1:D:330:MET:HB3	1.83	0.61
1:D:409:ARG:O	1:D:413:GLN:HG3	2.01	0.61
1:A:371:ASP:O	1:A:375:ILE:HG13	2.01	0.61
1:D:448:LYS:HZ2	1:D:449:LYS:HG2	1.66	0.61
1:A:370:LEU:HD11	1:A:426:LEU:HD21	1.81	0.61
1:B:230:SER:C	1:B:232:LYS:HG3	2.26	0.61
1:B:292:LYS:CE	2:F:696:LYS:HG2	2.31	0.61
1:B:463:ILE:O	1:B:464:TYR:CD1	2.54	0.61
1:C:384:CYS:O	1:C:401:GLN:HB2	2.01	0.61
1:C:453:ASP:CG	1:C:454:ALA:N	2.59	0.61
1:C:277:GLN:C	1:C:279:THR:H	2.06	0.61
1:C:288:THR:HA	1:C:309:LEU:HD11	1.81	0.61
1:C:325:MET:HG2	1:C:330:MET:HB3	1.83	0.60
1:A:257:LYS:HE2	1:A:261:ASN:HD22	1.63	0.60
1:D:459:LEU:C	1:D:461:GLN:H	2.09	0.60
1:A:412:LEU:HD22	1:A:422:LEU:HD23	1.84	0.60
1:B:343:PHE:O	1:B:347:LEU:CD1	2.50	0.60
1:C:258:LEU:HD13	1:C:263:ILE:HG21	1.82	0.60
2:H:685:LEU:HA	4:H:243:HOH:O	2.01	0.60
1:C:244:MET:HE3	1:C:268:ALA:CB	2.31	0.60
1:C:463:ILE:O	1:C:463:ILE:HG23	2.02	0.60
1:B:292:LYS:NZ	2:F:696:LYS:CG	2.65	0.60
1:A:244:MET:SD	1:A:268:ALA:CB	2.90	0.60
2:F:686:GLU:OE2	2:F:690:ARG:NH1	2.34	0.60
1:D:343:PHE:O	1:D:346:SER:OG	2.19	0.59
1:B:353:ASP:O	1:B:443:LEU:HD21	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:HD23	1:A:460:LEU:N	2.17	0.59
1:C:214:TYR:C	1:C:216:LYS:H	2.09	0.59
1:D:280:SER:O	1:D:284:VAL:HG23	2.03	0.59
1:B:462:GLU:C	1:B:464:TYR:H	2.10	0.59
1:A:268:ALA:HA	1:A:271:ARG:HE	1.67	0.59
1:D:302:LEU:O	1:D:306:VAL:HG23	2.02	0.59
1:B:314:TYR:CE1	3:B:776:471:H4A2	2.37	0.59
1:C:247:LEU:HD21	1:C:268:ALA:HB1	1.85	0.59
1:C:393:ASN:HB3	1:C:396:HIS:CE1	2.37	0.59
1:A:396:HIS:ND1	1:A:396:HIS:N	2.50	0.59
1:B:278:CYS:C	1:B:280:SER:H	2.08	0.59
1:C:297:PHE:HA	1:C:300:LEU:CD1	2.32	0.59
1:D:235:ASN:C	1:D:235:ASN:HD22	2.10	0.59
1:D:297:PHE:O	1:D:300:LEU:HD13	2.03	0.59
1:B:454:ALA:O	1:B:455:ALA:CB	2.51	0.59
2:F:686:GLU:O	2:F:690:ARG:HB2	2.03	0.59
1:B:251:GLU:CD	1:B:252:LYS:N	2.61	0.58
1:C:280:SER:C	1:C:282:GLU:N	2.60	0.58
1:C:268:ALA:O	1:C:271:ARG:N	2.36	0.58
1:C:443:LEU:HG	1:C:443:LEU:O	2.03	0.58
1:C:299:ASN:HA	2:F:697:TYR:HB2	1.85	0.58
1:C:460:LEU:CD2	1:C:464:TYR:CE2	2.86	0.58
1:D:288:THR:HA	1:D:309:LEU:HD11	1.84	0.58
1:A:396:HIS:HB3	1:A:399:LYS:HZ3	1.68	0.58
1:A:412:LEU:HD11	1:A:426:LEU:CD1	2.33	0.58
1:A:412:LEU:CD1	1:A:426:LEU:HD12	2.32	0.58
1:B:270:VAL:CG1	1:B:454:ALA:HB2	2.33	0.58
1:C:423:PHE:CZ	1:C:427:LEU:HD21	2.39	0.58
1:A:318:PHE:HA	1:A:321:LEU:HB2	1.85	0.58
1:C:345:LYS:C	1:C:352:CYS:HB2	2.28	0.58
1:D:271:ARG:C	1:D:273:PHE:H	2.10	0.58
1:D:308:LEU:HD11	1:D:397:ILE:HD13	1.84	0.58
1:D:349:LYS:HA	1:D:350:PRO:C	2.28	0.58
2:F:683:MET:HG3	2:F:684:GLY:H	1.69	0.58
1:C:209:ARG:NH2	1:C:293:ALA:C	2.62	0.58
1:A:269:GLU:CG	1:A:348:ARG:NH1	2.53	0.58
1:B:201:ALA:C	1:B:204:LYS:HE2	2.28	0.58
1:C:393:ASN:C	1:C:395:GLY:H	2.12	0.58
1:D:321:LEU:HD11	1:D:330:MET:HE1	1.86	0.58
1:A:244:MET:CE	1:A:268:ALA:HB2	2.32	0.58
1:B:324:VAL:HG13	1:B:324:VAL:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:PHE:CZ	1:B:427:LEU:HD21	2.38	0.58
1:A:277:GLN:C	1:A:279:THR:N	2.59	0.58
1:C:325:MET:HE2	1:C:359:PHE:CE1	2.39	0.58
1:C:358:LYS:HZ1	1:C:440:HIS:HB2	1.69	0.58
1:D:270:VAL:CG2	1:D:348:ARG:HH21	2.16	0.58
2:G:688:ILE:O	2:G:691:LYS:HG3	2.03	0.57
2:F:690:ARG:O	2:F:694:MET:HE3	2.04	0.57
1:A:217:ASN:O	1:A:286:GLU:HB3	2.05	0.57
1:A:230:SER:HB3	4:A:799:HOH:O	2.04	0.57
1:B:292:LYS:CE	2:F:696:LYS:HE2	2.34	0.57
1:C:363:MET:HE2	4:C:779:HOH:O	2.04	0.57
1:A:259:VAL:O	1:A:259:VAL:HG13	2.03	0.57
1:B:213:ALA:HB1	1:B:293:ALA:HB3	1.85	0.57
1:C:268:ALA:O	1:C:270:VAL:N	2.38	0.57
1:C:457:HIS:CD2	1:C:458:PRO:CD	2.87	0.57
1:D:209:ARG:CD	2:H:700:TRP:CZ3	2.83	0.57
1:D:351:PHE:C	1:D:353:ASP:N	2.62	0.57
1:B:450:THR:HG22	1:B:451:GLU:N	2.19	0.57
1:C:420:ILE:HD13	1:C:420:ILE:C	2.29	0.57
1:D:270:VAL:HG12	1:D:270:VAL:O	2.05	0.57
1:A:399:LYS:CG	1:A:400:MET:N	2.68	0.57
1:B:460:LEU:N	1:B:460:LEU:CD2	2.55	0.57
1:C:315:GLU:OE2	1:C:434:ARG:HG2	2.05	0.57
1:B:302:LEU:C	1:B:302:LEU:HD23	2.30	0.57
1:D:457:HIS:O	1:D:460:LEU:CD1	2.52	0.57
1:A:363:MET:HA	1:A:363:MET:CE	2.27	0.57
1:D:358:LYS:HD2	1:D:358:LYS:N	2.20	0.57
2:G:688:ILE:O	2:G:691:LYS:CG	2.53	0.57
1:B:251:GLU:OE1	1:B:251:GLU:N	2.38	0.56
1:D:301:ASP:HB3	1:D:303:ASN:H	1.70	0.56
1:B:459:LEU:C	1:B:460:LEU:HD23	2.29	0.56
1:A:263:ILE:H	1:A:263:ILE:CD1	2.17	0.56
1:A:263:ILE:HG22	1:A:266:LYS:HZ3	1.69	0.56
1:A:396:HIS:HB3	1:A:399:LYS:HZ2	1.68	0.56
1:C:218:PHE:HZ	1:C:287:LEU:HD23	1.70	0.56
1:C:297:PHE:O	1:C:300:LEU:CD1	2.52	0.56
1:A:276:CYS:O	1:A:280:SER:HB2	2.05	0.56
1:B:459:LEU:HD11	1:B:463:ILE:HD11	1.86	0.56
1:B:251:GLU:OE1	1:B:252:LYS:N	2.37	0.56
1:C:457:HIS:CG	1:C:458:PRO:HD3	2.40	0.56
1:B:301:ASP:C	1:B:303:ASN:N	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:VAL:HG23	1:D:348:ARG:HH21	1.68	0.56
1:B:456:LEU:H	1:B:456:LEU:CD2	1.93	0.56
1:C:231:GLY:C	1:C:233:ALA:N	2.63	0.56
3:D:778:471:H4A1	4:D:779:HOH:O	2.05	0.56
2:E:683:MET:HG3	2:E:684:GLY:N	2.19	0.56
2:G:685:LEU:H	2:G:685:LEU:HD23	1.70	0.56
1:C:461:GLN:HE22	1:C:465:ARG:HH11	1.52	0.56
1:A:238:PRO:HA	1:A:336:ASN:O	2.05	0.56
1:C:467:MET:O	1:C:468:TYR:CG	2.59	0.55
2:H:683:MET:HG3	2:H:684:GLY:N	2.21	0.55
1:A:232:LYS:O	1:A:233:ALA:HB3	2.07	0.55
1:C:269:GLU:HB2	1:C:351:PHE:CD2	2.42	0.55
2:H:686:GLU:HA	2:H:689:ILE:HG23	1.88	0.55
1:B:201:ALA:HA	1:B:204:LYS:CD	2.37	0.55
1:D:252:LYS:HA	1:D:258:LEU:HD13	1.89	0.55
1:B:247:LEU:O	1:B:251:GLU:HG3	2.07	0.55
1:D:382:ILE:HD12	1:D:382:ILE:C	2.32	0.55
1:A:374:ASP:OD2	1:A:416:HIS:CE1	2.54	0.55
1:C:242:HIS:CE1	1:C:243:ASP:OD2	2.60	0.55
1:C:396:HIS:O	1:C:400:MET:HB2	2.07	0.55
1:A:247:LEU:O	1:A:247:LEU:HG	2.04	0.55
1:B:209:ARG:HD2	2:F:700:TRP:CZ3	2.42	0.55
1:B:457:HIS:C	1:B:459:LEU:N	2.54	0.55
1:C:235:ASN:O	1:C:236:ASN:HB3	2.06	0.55
1:D:259:VAL:O	1:D:260:ALA:HB2	2.06	0.55
1:A:340:THR:O	1:A:344:LEU:HD12	2.07	0.55
1:D:351:PHE:O	1:D:354:ILE:N	2.31	0.55
1:A:269:GLU:HB2	1:A:351:PHE:CE2	2.42	0.54
1:B:427:LEU:CD2	1:B:430:MET:HE2	2.37	0.54
1:C:346:SER:O	1:C:347:LEU:HD23	2.07	0.54
1:D:394:VAL:O	1:D:394:VAL:CG1	2.53	0.54
1:A:422:LEU:O	1:A:425:LYS:HB2	2.07	0.54
1:A:429:LYS:C	1:A:431:ALA:N	2.65	0.54
1:D:370:LEU:HD11	1:D:426:LEU:HD21	1.88	0.54
1:A:409:ARG:HG2	1:A:413:GLN:NE2	2.22	0.54
1:A:448:LYS:O	1:A:452:SER:OG	2.19	0.54
2:E:697:TYR:O	2:E:697:TYR:CD1	2.55	0.54
1:D:300:LEU:HD23	1:D:397:ILE:HD11	1.90	0.54
1:B:235:ASN:OD1	1:B:236:ASN:N	2.40	0.54
1:B:457:HIS:O	1:B:459:LEU:N	2.41	0.54
1:B:292:LYS:NZ	2:F:696:LYS:HG2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:PHE:HB3	1:B:424:PRO:CD	2.38	0.54
1:A:263:ILE:HD13	1:A:263:ILE:N	2.23	0.54
1:A:263:ILE:CG2	1:A:266:LYS:NZ	2.71	0.54
1:A:457:HIS:ND1	1:A:458:PRO:HD2	2.22	0.54
1:B:257:LYS:O	1:B:257:LYS:HG2	2.07	0.54
1:B:297:PHE:HA	1:B:400:MET:HE1	1.88	0.54
1:C:209:ARG:HH22	1:C:293:ALA:CB	2.12	0.54
1:D:350:PRO:O	1:D:353:ASP:OD2	2.26	0.54
1:D:444:VAL:O	1:D:446:ILE:N	2.33	0.54
1:A:257:LYS:O	1:A:257:LYS:CG	2.56	0.54
1:B:280:SER:O	1:B:284:VAL:HG23	2.08	0.54
1:C:363:MET:HA	1:C:363:MET:CE	2.38	0.54
1:C:421:PHE:O	1:C:425:LYS:HB2	2.08	0.54
2:F:689:ILE:HG13	2:F:693:LEU:HD22	1.90	0.54
1:A:273:PHE:CD2	1:A:273:PHE:C	2.86	0.54
1:C:220:MET:HE1	1:C:228:ILE:HD12	1.90	0.54
1:D:363:MET:HE3	1:D:363:MET:HA	1.91	0.54
2:E:682:ASN:O	2:E:683:MET:CB	2.56	0.54
1:B:279:THR:O	1:B:279:THR:HG22	2.08	0.53
1:D:445:GLN:O	1:D:446:ILE:HG13	2.08	0.53
1:C:299:ASN:O	1:C:300:LEU:C	2.51	0.53
1:C:348:ARG:O	1:C:351:PHE:HB2	2.07	0.53
1:C:460:LEU:HD23	1:C:464:TYR:CD2	2.43	0.53
1:C:211:TYR:CZ	1:C:215:LEU:HD11	2.43	0.53
1:D:351:PHE:C	1:D:353:ASP:H	2.16	0.53
1:A:379:VAL:O	1:A:383:ILE:HG13	2.08	0.53
1:B:292:LYS:HZ1	2:F:696:LYS:HE3	1.73	0.53
1:C:300:LEU:H	1:C:300:LEU:CD1	1.94	0.53
1:C:370:LEU:HD11	1:C:426:LEU:HD21	1.90	0.53
1:A:279:THR:HG21	4:A:798:HOH:O	2.08	0.53
1:A:345:LYS:O	1:A:345:LYS:CG	2.56	0.53
1:C:463:ILE:O	1:C:464:TYR:HD2	1.92	0.53
1:D:457:HIS:CD2	1:D:459:LEU:N	2.77	0.53
1:A:220:MET:HE1	1:A:228:ILE:HD12	1.90	0.53
1:A:344:LEU:O	1:A:347:LEU:HG	2.09	0.53
1:C:209:ARG:NH2	1:C:293:ALA:O	2.42	0.53
1:C:247:LEU:CD1	1:C:272:ILE:HD11	2.39	0.53
1:B:439:GLU:O	1:B:443:LEU:HB3	2.08	0.53
1:C:288:THR:CG2	2:G:693:LEU:HD13	2.39	0.53
1:D:457:HIS:HD2	1:D:459:LEU:CA	2.22	0.53
1:C:237:PRO:HB2	1:C:238:PRO:CD	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:LEU:HD23	1:A:459:LEU:C	2.33	0.52
1:B:301:ASP:O	1:B:303:ASN:N	2.42	0.52
1:C:280:SER:C	1:C:282:GLU:H	2.17	0.52
1:A:244:MET:HE1	1:A:268:ALA:CB	2.36	0.52
1:B:258:LEU:HD22	1:B:263:ILE:HB	1.90	0.52
1:B:453:ASP:CG	1:B:454:ALA:H	2.17	0.52
1:D:255:VAL:N	1:D:258:LEU:HD11	2.17	0.52
1:A:354:ILE:O	1:A:357:PRO:HD2	2.09	0.52
1:C:280:SER:O	1:C:282:GLU:N	2.43	0.52
1:B:269:GLU:OE1	1:B:348:ARG:N	2.43	0.52
1:B:338:PHE:CD1	1:B:338:PHE:C	2.88	0.52
1:D:269:GLU:HB3	1:D:347:LEU:HD22	1.90	0.52
2:F:695:GLY:HA2	4:F:242:HOH:O	2.09	0.52
1:A:388:ARG:O	1:A:391:LEU:HG	2.10	0.52
1:C:420:ILE:HD11	1:C:421:PHE:CD2	2.45	0.52
1:D:271:ARG:C	1:D:273:PHE:N	2.67	0.52
1:C:444:VAL:C	1:C:446:ILE:H	2.17	0.52
1:A:275:CYS:O	1:A:278:CYS:N	2.42	0.52
2:H:686:GLU:O	2:H:690:ARG:HB2	2.10	0.52
1:A:257:LYS:O	1:A:261:ASN:HB2	2.09	0.52
1:B:355:MET:HE2	3:B:776:471:HC1M	1.92	0.52
1:C:247:LEU:HD13	1:C:272:ILE:HD11	1.92	0.52
1:C:279:THR:HG22	1:C:279:THR:O	2.09	0.51
1:C:293:ALA:O	1:C:294:ILE:C	2.53	0.51
1:D:412:LEU:HD11	1:D:426:LEU:CD1	2.40	0.51
1:D:448:LYS:HZ2	1:D:449:LYS:CG	2.24	0.51
1:B:235:ASN:ND2	4:B:880:HOH:O	2.43	0.51
1:C:306:VAL:HA	2:G:689:ILE:HD11	1.92	0.51
1:B:230:SER:O	1:B:231:GLY:C	2.53	0.51
1:B:370:LEU:HD11	1:B:426:LEU:HD21	1.92	0.51
1:D:255:VAL:HB	1:D:258:LEU:CD1	2.40	0.51
2:H:685:LEU:HD23	2:H:685:LEU:N	2.26	0.51
1:B:412:LEU:HG	1:B:422:LEU:HD13	1.93	0.51
1:C:214:TYR:C	1:C:216:LYS:N	2.68	0.51
1:D:230:SER:O	1:D:232:LYS:HD3	2.09	0.51
1:A:312:GLY:O	1:A:382:ILE:HD11	2.11	0.51
1:B:255:VAL:HG11	1:B:258:LEU:HG	1.91	0.51
1:B:340:THR:HG22	1:B:343:PHE:H	1.75	0.51
1:C:276:CYS:SG	3:C:777:471:H3A1	2.51	0.51
1:D:255:VAL:O	1:D:258:LEU:HD12	2.10	0.51
1:D:356:GLU:N	1:D:357:PRO:CD	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:VAL:HG11	1:B:454:ALA:HB2	1.92	0.51
1:C:269:GLU:HB2	1:C:351:PHE:CE2	2.45	0.51
1:B:412:LEU:CD2	1:B:426:LEU:HD12	2.39	0.51
1:D:262:GLY:O	1:D:266:LYS:HE3	2.11	0.51
1:A:301:ASP:OD1	1:A:303:ASN:N	2.44	0.50
1:A:375:ILE:O	1:A:379:VAL:HG23	2.11	0.50
1:A:422:LEU:HA	1:A:425:LYS:HD2	1.93	0.50
1:D:288:THR:CG2	2:H:693:LEU:HD13	2.41	0.50
1:D:447:ILE:O	1:D:447:ILE:HG22	2.11	0.50
1:B:338:PHE:HD1	1:B:338:PHE:O	1.95	0.50
1:C:207:ALA:HB2	1:C:407:VAL:HG13	1.93	0.50
1:D:373:SER:HG	1:D:411:HIS:CE1	2.29	0.50
1:D:309:LEU:O	1:D:313:VAL:HB	2.11	0.50
1:A:299:ASN:O	1:A:300:LEU:C	2.53	0.50
1:A:420:ILE:CD1	1:A:421:PHE:N	2.71	0.50
1:B:246:THR:C	1:B:248:CYS:N	2.68	0.50
1:B:269:GLU:OE1	1:B:347:LEU:HB3	2.11	0.50
1:B:276:CYS:SG	3:B:776:471:H3A1	2.51	0.50
1:B:355:MET:HG2	3:B:776:471:HC1L	1.93	0.50
1:C:378:PHE:HE1	1:C:430:MET:HG3	1.76	0.50
1:C:412:LEU:CD1	1:C:422:LEU:HG	2.41	0.50
1:D:248:CYS:O	1:D:252:LYS:HB2	2.11	0.50
1:A:421:PHE:C	1:A:424:PRO:HD2	2.36	0.50
1:A:429:LYS:C	1:A:431:ALA:H	2.19	0.50
1:C:301:ASP:O	1:C:302:LEU:C	2.55	0.50
1:D:409:ARG:NH1	1:D:409:ARG:CB	2.74	0.50
2:E:685:LEU:C	2:E:687:ALA:N	2.69	0.50
1:A:279:THR:HG22	1:A:279:THR:O	2.12	0.50
1:A:457:HIS:CE1	1:A:458:PRO:HD2	2.47	0.50
1:C:394:VAL:O	1:C:394:VAL:CG1	2.59	0.50
1:D:358:LYS:HD2	1:D:358:LYS:H	1.76	0.50
1:D:393:ASN:C	1:D:395:GLY:H	2.20	0.50
1:D:409:ARG:NH1	1:D:409:ARG:HB2	2.27	0.50
2:F:696:LYS:C	2:F:696:LYS:CD	2.82	0.50
1:B:434:ARG:NH2	4:B:805:HOH:O	2.29	0.50
1:B:460:LEU:O	1:B:462:GLU:O	2.30	0.50
1:C:438:THR:CG2	1:C:439:GLU:N	2.75	0.50
1:C:462:GLU:O	1:C:463:ILE:HG22	2.11	0.50
2:H:683:MET:CG	2:H:684:GLY:H	2.25	0.50
1:C:276:CYS:SG	3:C:777:471:HC1M	2.51	0.49
1:D:297:PHE:HA	1:D:300:LEU:CD1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:686:GLU:O	2:G:690:ARG:HB2	2.12	0.49
1:A:270:VAL:HG12	1:A:270:VAL:O	2.11	0.49
1:A:275:CYS:O	1:A:277:GLN:N	2.45	0.49
1:C:354:ILE:O	1:C:357:PRO:HD2	2.12	0.49
1:D:251:GLU:O	1:D:258:LEU:HD13	2.12	0.49
1:A:258:LEU:HD23	1:A:258:LEU:N	2.27	0.49
1:C:391:LEU:HB2	1:C:394:VAL:HG23	1.94	0.49
1:D:231:GLY:O	1:D:232:LYS:C	2.54	0.49
1:A:351:PHE:O	1:A:353:ASP:N	2.46	0.49
1:B:244:MET:O	1:B:248:CYS:HB2	2.12	0.49
1:D:412:LEU:CD1	1:D:426:LEU:HD12	2.40	0.49
1:A:356:GLU:N	1:A:357:PRO:CD	2.76	0.49
1:A:467:MET:HA	1:A:467:MET:CE	2.39	0.49
1:D:309:LEU:CB	2:H:689:ILE:HD12	2.43	0.49
1:D:384:CYS:HB3	1:D:400:MET:HE2	1.94	0.49
1:D:457:HIS:HD2	1:D:459:LEU:N	2.10	0.49
1:D:460:LEU:HD12	1:D:460:LEU:N	2.18	0.49
1:A:385:CYS:SG	1:A:388:ARG:NE	2.85	0.49
1:B:248:CYS:HA	1:B:251:GLU:CD	2.38	0.49
1:B:434:ARG:O	1:B:437:VAL:HG12	2.13	0.49
1:C:355:MET:HB2	4:C:806:HOH:O	2.11	0.49
1:D:420:ILE:HD11	1:D:421:PHE:CZ	2.47	0.49
1:B:230:SER:O	1:B:232:LYS:CE	2.57	0.49
1:C:225:ALA:O	1:C:229:LEU:HD12	2.13	0.49
1:D:235:ASN:CG	1:D:235:ASN:O	2.55	0.49
1:D:396:HIS:O	1:D:400:MET:N	2.44	0.49
1:B:248:CYS:C	1:B:251:GLU:OE1	2.55	0.49
1:B:445:GLN:HA	1:B:445:GLN:NE2	2.12	0.49
1:C:446:ILE:O	1:C:446:ILE:CG2	2.60	0.49
1:D:257:LYS:HG2	1:D:257:LYS:O	2.11	0.49
1:A:244:MET:SD	1:A:268:ALA:HB3	2.52	0.49
1:B:338:PHE:CD1	1:B:338:PHE:O	2.66	0.49
1:C:325:MET:HE2	1:C:359:PHE:CD1	2.48	0.49
1:D:251:GLU:O	1:D:258:LEU:CD1	2.61	0.49
1:A:209:ARG:HD3	2:E:700:TRP:CH2	2.47	0.48
1:D:455:ALA:C	1:D:456:LEU:HD13	2.38	0.48
2:H:683:MET:O	2:H:685:LEU:HD23	2.13	0.48
1:B:343:PHE:O	1:B:343:PHE:CD1	2.66	0.48
1:C:246:THR:HA	1:C:249:MET:HE3	1.95	0.48
1:C:412:LEU:HD11	1:C:422:LEU:HG	1.95	0.48
1:D:272:ILE:O	1:D:272:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:HG23	1:A:266:LYS:NZ	2.28	0.48
1:C:229:LEU:HD22	1:C:326:ASN:ND2	2.28	0.48
1:C:247:LEU:CD2	1:C:272:ILE:HD11	2.43	0.48
1:D:345:LYS:C	1:D:352:CYS:HB3	2.39	0.48
2:E:691:LYS:O	2:E:691:LYS:HG2	2.13	0.48
1:B:391:LEU:HB2	1:B:394:VAL:HG23	1.96	0.48
1:D:409:ARG:HH11	1:D:409:ARG:HB3	1.79	0.48
1:C:299:ASN:O	1:C:300:LEU:O	2.31	0.48
1:C:363:MET:HE3	1:C:363:MET:CA	2.39	0.48
1:D:420:ILE:HD11	1:D:421:PHE:CD1	2.49	0.48
1:D:444:VAL:C	1:D:446:ILE:H	2.21	0.48
2:F:690:ARG:O	2:F:694:MET:CE	2.62	0.48
1:A:237:PRO:HB2	1:A:238:PRO:HD2	1.95	0.48
1:B:437:VAL:CG1	1:B:438:THR:N	2.76	0.48
1:B:462:GLU:C	1:B:464:TYR:N	2.72	0.48
1:D:311:TYR:CZ	1:D:389:PRO:HG2	2.48	0.48
2:F:685:LEU:N	2:F:685:LEU:HD23	2.29	0.48
1:A:209:ARG:HD3	2:E:700:TRP:CZ3	2.49	0.48
1:A:457:HIS:CG	1:A:458:PRO:CD	2.92	0.48
1:B:257:LYS:O	1:B:261:ASN:HB2	2.14	0.48
1:B:446:ILE:O	1:B:446:ILE:CG2	2.59	0.48
1:D:205:SER:O	1:D:209:ARG:HB2	2.13	0.48
1:D:274:HIS:O	1:D:277:GLN:N	2.31	0.48
1:D:460:LEU:CD1	1:D:460:LEU:N	2.76	0.48
1:B:209:ARG:HD2	2:F:700:TRP:HZ3	1.77	0.48
1:C:230:SER:C	1:C:232:LYS:N	2.69	0.48
1:C:291:ALA:C	1:C:293:ALA:N	2.71	0.48
1:C:457:HIS:C	1:C:459:LEU:H	2.22	0.48
1:D:409:ARG:CB	1:D:409:ARG:HH11	2.26	0.48
1:A:237:PRO:CB	1:A:238:PRO:HD2	2.44	0.47
1:C:268:ALA:C	1:C:270:VAL:H	2.21	0.47
1:C:301:ASP:O	1:C:304:ASP:N	2.47	0.47
1:D:445:GLN:C	1:D:446:ILE:HG13	2.38	0.47
1:D:446:ILE:HG22	1:D:446:ILE:O	2.12	0.47
1:B:242:HIS:NE2	1:B:246:THR:HG21	2.29	0.47
1:B:287:LEU:HD22	1:B:383:ILE:HD11	1.97	0.47
1:C:258:LEU:HD13	1:C:263:ILE:CG2	2.45	0.47
1:C:288:THR:HG23	1:C:309:LEU:CD1	2.43	0.47
1:C:289:GLU:OE1	1:C:289:GLU:HA	2.14	0.47
1:D:331:LEU:HD23	1:D:338:PHE:HD2	1.79	0.47
1:D:384:CYS:SG	1:D:400:MET:CE	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ASN:HB3	1:A:396:HIS:ND1	2.29	0.47
1:B:230:SER:O	1:B:232:LYS:CG	2.55	0.47
1:B:348:ARG:O	1:B:351:PHE:HD2	1.96	0.47
1:C:242:HIS:HB3	1:C:340:THR:HG21	1.95	0.47
1:C:396:HIS:O	1:C:400:MET:CB	2.62	0.47
1:C:423:PHE:HB3	1:C:424:PRO:CD	2.44	0.47
1:D:396:HIS:CG	4:D:838:HOH:O	2.66	0.47
1:A:212:GLU:OE1	2:E:700:TRP:CH2	2.67	0.47
1:B:214:TYR:CD1	1:B:214:TYR:C	2.92	0.47
1:B:292:LYS:HZ1	2:F:696:LYS:HE2	1.77	0.47
1:C:422:LEU:HA	1:C:425:LYS:HB2	1.97	0.47
1:D:443:LEU:HD12	1:D:443:LEU:O	2.14	0.47
1:A:302:LEU:C	1:A:302:LEU:HD12	2.39	0.47
1:B:349:LYS:HG3	1:B:350:PRO:HA	1.95	0.47
1:B:427:LEU:HD22	1:B:430:MET:CE	2.45	0.47
1:C:207:ALA:HB2	1:C:407:VAL:CG1	2.44	0.47
1:C:463:ILE:HG23	1:C:464:TYR:HD2	1.79	0.47
1:C:465:ARG:HH11	1:C:465:ARG:HG3	1.79	0.47
1:D:351:PHE:O	1:D:352:CYS:C	2.58	0.47
1:A:301:ASP:O	1:A:304:ASP:N	2.45	0.47
1:B:268:ALA:HB1	1:B:271:ARG:NH2	2.30	0.47
1:C:382:ILE:HG22	1:C:430:MET:HE2	1.96	0.47
1:A:435:GLN:O	1:A:439:GLU:HG3	2.15	0.47
1:B:254:LEU:CD2	3:B:776:471:HC3M	2.44	0.47
1:B:270:VAL:CG1	1:B:454:ALA:HB3	2.42	0.47
1:B:457:HIS:ND1	1:B:459:LEU:N	2.62	0.47
1:D:462:GLU:O	1:D:463:ILE:HG13	2.14	0.47
2:E:700:TRP:O	2:E:700:TRP:CG	2.67	0.47
1:B:437:VAL:HG12	1:B:438:THR:N	2.29	0.47
1:C:208:LYS:O	1:C:208:LYS:HG2	2.11	0.47
1:D:264:GLN:H	1:D:264:GLN:NE2	2.12	0.47
1:A:220:MET:HE1	1:A:228:ILE:CD1	2.45	0.47
1:A:267:GLU:OE1	1:A:348:ARG:NH1	2.48	0.47
1:B:288:THR:HA	1:B:309:LEU:HD11	1.96	0.47
1:C:393:ASN:C	1:C:395:GLY:N	2.70	0.47
1:D:230:SER:O	1:D:232:LYS:N	2.47	0.47
1:C:282:GLU:OE1	1:C:282:GLU:HA	2.15	0.46
1:C:446:ILE:C	1:C:447:ILE:HG13	2.39	0.46
1:C:457:HIS:O	1:C:460:LEU:HD12	2.15	0.46
1:D:290:PHE:HE2	1:D:379:VAL:HG12	1.80	0.46
1:A:315:GLU:CB	1:A:382:ILE:HD13	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ASP:C	1:B:303:ASN:H	2.22	0.46
1:B:349:LYS:HA	1:B:351:PHE:H	1.80	0.46
1:D:242:HIS:HE1	1:D:243:ASP:OD2	1.94	0.46
1:A:461:GLN:NE2	1:A:461:GLN:N	2.63	0.46
1:C:247:LEU:HD12	1:C:247:LEU:O	2.16	0.46
1:D:425:LYS:O	1:D:429:LYS:HG2	2.15	0.46
1:C:263:ILE:HG12	1:C:266:LYS:NZ	2.30	0.46
1:D:259:VAL:O	1:D:259:VAL:HG13	2.15	0.46
1:C:396:HIS:CE1	4:C:785:HOH:O	2.68	0.46
1:A:222:LYS:O	1:A:226:ARG:HG2	2.15	0.46
1:C:300:LEU:N	1:C:300:LEU:CD1	2.63	0.46
1:A:269:GLU:OE1	1:A:348:ARG:HG2	2.16	0.46
1:A:273:PHE:HZ	1:A:454:ALA:O	1.90	0.46
1:A:457:HIS:C	1:A:459:LEU:H	2.24	0.46
1:B:445:GLN:C	1:B:447:ILE:N	2.73	0.46
1:D:235:ASN:ND2	1:D:237:PRO:HD3	2.30	0.46
1:A:298:ALA:HA	1:A:305:GLN:NE2	2.31	0.46
1:B:309:LEU:HB3	2:F:689:ILE:HD12	1.97	0.46
1:C:244:MET:HA	1:C:247:LEU:HB3	1.98	0.46
1:C:248:CYS:O	1:C:252:LYS:HB2	2.16	0.46
1:C:450:THR:O	1:C:450:THR:CG2	2.64	0.46
2:E:685:LEU:H	2:E:685:LEU:CD2	1.89	0.46
1:A:320:MET:C	1:A:322:SER:N	2.73	0.46
1:A:460:LEU:CD2	2:E:688:ILE:HD11	2.46	0.46
1:D:229:LEU:CD2	1:D:338:PHE:HE2	2.29	0.46
1:D:465:ARG:HG3	1:D:465:ARG:NH1	2.29	0.46
1:A:252:LYS:HD3	1:A:259:VAL:HG23	1.98	0.46
1:B:201:ALA:O	1:B:204:LYS:CE	2.60	0.46
1:B:259:VAL:HG22	1:B:259:VAL:O	2.16	0.46
1:B:348:ARG:NH2	1:B:351:PHE:CE2	2.75	0.46
1:C:391:LEU:HD22	1:C:397:ILE:CD1	2.46	0.46
1:D:248:CYS:O	1:D:252:LYS:CB	2.64	0.46
1:A:393:ASN:C	1:A:395:GLY:H	2.24	0.45
1:C:209:ARG:NH2	1:C:293:ALA:CB	2.75	0.45
1:B:292:LYS:HZ1	2:F:696:LYS:CG	2.29	0.45
1:C:460:LEU:HA	1:C:462:GLU:O	2.17	0.45
1:A:396:HIS:O	1:A:400:MET:HB2	2.16	0.45
1:B:447:ILE:O	1:B:447:ILE:HG22	2.15	0.45
1:C:358:LYS:NZ	1:C:440:HIS:HD2	2.14	0.45
1:C:378:PHE:CE1	1:C:430:MET:HG3	2.51	0.45
1:D:432:ASP:O	1:D:435:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:ARG:O	1:D:465:ARG:HD3	2.16	0.45
2:E:683:MET:O	2:E:685:LEU:CD2	2.64	0.45
1:B:348:ARG:HG2	1:B:348:ARG:HH11	1.80	0.45
1:B:451:GLU:C	1:B:453:ASP:OD1	2.57	0.45
1:C:307:THR:HA	1:C:310:LYS:HD3	1.98	0.45
1:D:294:ILE:O	1:D:296:GLY:N	2.50	0.45
1:C:255:VAL:HB	1:C:258:LEU:HG	1.98	0.45
1:D:274:HIS:O	1:D:277:GLN:CB	2.61	0.45
2:E:685:LEU:C	2:E:687:ALA:H	2.24	0.45
2:E:697:TYR:O	2:E:698:ASP:CB	2.57	0.45
1:C:248:CYS:C	1:C:250:ALA:N	2.74	0.45
1:C:252:LYS:NZ	1:C:259:VAL:HG23	2.31	0.45
1:D:348:ARG:CG	1:D:349:LYS:H	2.28	0.45
2:G:688:ILE:CD1	2:G:689:ILE:HG22	2.46	0.45
1:B:255:VAL:HG12	1:B:257:LYS:H	1.81	0.45
1:B:427:LEU:HD22	1:B:430:MET:HE2	1.97	0.45
1:C:280:SER:O	1:C:283:THR:N	2.50	0.45
1:B:221:ASN:OD1	1:B:224:LYS:HG3	2.16	0.45
1:C:245:GLU:O	1:C:248:CYS:HB2	2.17	0.45
1:C:463:ILE:CG2	1:C:464:TYR:HD2	2.29	0.45
1:C:247:LEU:CD2	1:C:268:ALA:HB1	2.47	0.45
1:D:257:LYS:HZ1	1:D:263:ILE:HD11	1.82	0.45
1:A:257:LYS:HE2	1:A:261:ASN:HD21	1.75	0.45
1:B:325:MET:HG2	1:B:330:MET:CB	2.46	0.45
1:C:462:GLU:H	1:C:462:GLU:HG2	1.56	0.45
2:F:697:TYR:N	2:F:697:TYR:CD1	2.85	0.44
2:G:685:LEU:HD23	2:G:685:LEU:N	2.32	0.44
1:B:324:VAL:O	1:B:324:VAL:CG1	2.66	0.44
1:D:208:LYS:O	1:D:212:GLU:HG2	2.17	0.44
1:D:249:MET:O	1:D:250:ALA:C	2.60	0.44
1:D:317:ILE:O	1:D:321:LEU:HB2	2.17	0.44
1:A:301:ASP:O	1:A:302:LEU:C	2.60	0.44
1:C:250:ALA:C	1:C:252:LYS:N	2.76	0.44
1:C:268:ALA:HA	1:C:271:ARG:NH1	2.33	0.44
1:D:270:VAL:O	1:D:270:VAL:CG1	2.65	0.44
1:D:455:ALA:O	1:D:456:LEU:HD13	2.17	0.44
1:B:304:ASP:OD1	1:B:391:LEU:HA	2.16	0.44
1:C:250:ALA:C	1:C:252:LYS:H	2.26	0.44
1:C:382:ILE:HG13	1:C:383:ILE:N	2.33	0.44
1:C:325:MET:HG2	1:C:330:MET:CB	2.48	0.44
1:A:269:GLU:HB2	1:A:351:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:MET:HE2	1:A:359:PHE:CE2	2.52	0.44
1:B:418:ASP:HB2	4:B:849:HOH:O	2.17	0.44
1:D:353:ASP:O	1:D:357:PRO:CD	2.65	0.44
2:E:691:LYS:HE2	2:E:691:LYS:HB3	1.74	0.44
1:C:284:VAL:HG12	1:C:284:VAL:O	2.18	0.44
1:C:297:PHE:C	1:C:300:LEU:CD1	2.91	0.44
1:C:408:LEU:HD23	1:C:423:PHE:HE1	1.82	0.44
1:C:438:THR:HG22	1:C:439:GLU:HG3	2.00	0.44
1:C:460:LEU:HB3	1:C:464:TYR:CG	2.53	0.44
1:D:383:ILE:C	1:D:385:CYS:H	2.25	0.44
1:B:427:LEU:HD23	1:B:430:MET:HE2	1.98	0.44
1:C:343:PHE:O	1:C:343:PHE:CG	2.71	0.44
1:D:354:ILE:O	1:D:357:PRO:HD2	2.17	0.44
1:B:208:LYS:O	1:B:208:LYS:HG3	2.18	0.43
1:B:309:LEU:CB	2:F:689:ILE:HD12	2.48	0.43
1:C:426:LEU:C	1:C:428:GLN:N	2.76	0.43
1:C:426:LEU:O	1:C:429:LYS:N	2.51	0.43
1:D:223:VAL:HG23	1:D:372:ASP:OD2	2.18	0.43
1:D:457:HIS:C	1:D:459:LEU:N	2.68	0.43
1:A:257:LYS:CG	1:A:261:ASN:ND2	2.81	0.43
1:A:419:ASP:CB	1:A:422:LEU:HB2	2.45	0.43
1:C:202:ASP:C	1:C:204:LYS:H	2.26	0.43
1:A:441:ALA:O	1:A:445:GLN:HG3	2.18	0.43
1:B:411:HIS:O	1:B:415:ASN:HB2	2.17	0.43
1:C:245:GLU:HG2	1:C:249:MET:HE2	2.01	0.43
1:D:307:THR:HG21	1:D:391:LEU:CD2	2.48	0.43
1:D:392:LEU:HD13	1:D:393:ASN:ND2	2.33	0.43
1:B:301:ASP:O	1:B:302:LEU:C	2.62	0.43
1:C:247:LEU:HD22	1:C:272:ILE:HD11	1.99	0.43
1:D:459:LEU:C	1:D:461:GLN:N	2.75	0.43
1:A:257:LYS:O	1:A:258:LEU:HD23	2.16	0.43
1:B:421:PHE:O	1:B:425:LYS:HG3	2.18	0.43
1:B:428:GLN:HB2	4:B:785:HOH:O	2.17	0.43
1:C:211:TYR:O	1:C:214:TYR:HB3	2.18	0.43
1:A:268:ALA:O	1:A:269:GLU:C	2.62	0.43
1:C:301:ASP:O	1:C:303:ASN:N	2.52	0.43
1:C:465:ARG:O	1:C:467:MET:N	2.51	0.43
1:D:224:LYS:O	1:D:228:ILE:HG13	2.18	0.43
1:D:254:LEU:CD2	3:D:778:471:HC3M	2.48	0.43
1:D:399:LYS:HB2	1:D:399:LYS:HE3	1.70	0.43
1:A:460:LEU:HD22	2:E:688:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:LEU:CD1	1:B:463:ILE:HD11	2.46	0.43
1:C:230:SER:C	1:C:232:LYS:H	2.12	0.43
1:D:355:MET:C	1:D:357:PRO:HD2	2.44	0.43
1:B:238:PRO:HA	1:B:336:ASN:O	2.19	0.43
1:B:459:LEU:CD1	1:B:459:LEU:C	2.91	0.43
1:C:264:GLN:O	1:C:265:ASN:HB2	2.18	0.43
2:F:690:ARG:HG2	4:F:270:HOH:O	2.18	0.43
1:D:345:LYS:HA	1:D:352:CYS:CA	2.47	0.43
1:D:393:ASN:HB3	1:D:396:HIS:CD2	2.54	0.43
1:A:258:LEU:HD13	1:A:263:ILE:HB	2.00	0.43
1:A:396:HIS:C	1:A:399:LYS:HG2	2.43	0.43
1:B:237:PRO:CB	1:B:238:PRO:HD2	2.49	0.43
1:B:288:THR:HG21	2:F:692:ALA:HB3	2.00	0.43
2:H:700:TRP:CD2	2:H:700:TRP:C	2.97	0.43
1:C:349:LYS:HB3	1:C:349:LYS:HE3	1.52	0.42
1:D:207:ALA:HB2	1:D:407:VAL:CG1	2.49	0.42
1:D:412:LEU:HD23	1:D:412:LEU:HA	1.88	0.42
1:A:364:LYS:O	1:A:367:ALA:HB3	2.19	0.42
1:B:445:GLN:O	1:B:447:ILE:N	2.48	0.42
1:C:269:GLU:CB	1:C:351:PHE:HD2	2.33	0.42
1:C:444:VAL:C	1:C:446:ILE:N	2.76	0.42
1:A:202:ASP:OD1	1:A:202:ASP:N	2.40	0.42
1:B:460:LEU:HB3	1:B:464:TYR:HE2	1.84	0.42
1:C:345:LYS:O	1:C:352:CYS:HB2	2.18	0.42
1:D:255:VAL:HB	1:D:258:LEU:HD11	2.00	0.42
1:D:334:TYR:HE1	4:D:812:HOH:O	1.99	0.42
1:D:459:LEU:HD12	1:D:459:LEU:C	2.37	0.42
1:B:243:ASP:O	1:B:245:GLU:N	2.52	0.42
1:B:301:ASP:O	1:B:304:ASP:N	2.53	0.42
1:C:465:ARG:HD3	1:C:465:ARG:C	2.43	0.42
1:D:353:ASP:O	1:D:357:PRO:CG	2.67	0.42
1:A:212:GLU:OE1	2:E:700:TRP:CZ3	2.71	0.42
1:A:345:LYS:HA	1:A:352:CYS:HB2	2.00	0.42
1:B:212:GLU:OE1	2:F:700:TRP:CH2	2.73	0.42
1:B:445:GLN:NE2	1:B:448:LYS:HD2	2.35	0.42
1:C:353:ASP:O	1:C:443:LEU:HD21	2.20	0.42
2:F:697:TYR:N	2:F:697:TYR:HD1	2.18	0.42
1:A:446:ILE:O	1:A:450:THR:HB	2.19	0.42
1:C:250:ALA:O	1:C:252:LYS:N	2.53	0.42
1:C:301:ASP:C	1:C:303:ASN:N	2.78	0.42
1:A:370:LEU:HB3	1:A:374:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:VAL:O	1:B:281:VAL:HG12	2.19	0.42
1:C:252:LYS:HZ1	1:C:259:VAL:CG2	2.32	0.42
1:D:371:ASP:OD1	1:D:371:ASP:C	2.63	0.42
1:A:290:PHE:O	1:A:294:ILE:HG13	2.19	0.42
1:A:308:LEU:HD11	1:A:397:ILE:HD13	2.00	0.42
1:A:412:LEU:HD22	1:A:422:LEU:CD2	2.49	0.42
1:B:247:LEU:HD21	1:B:272:ILE:HG12	2.00	0.42
1:B:313:VAL:HG11	2:F:685:LEU:HD11	2.00	0.42
1:B:463:ILE:O	1:B:464:TYR:HD1	2.03	0.42
1:C:269:GLU:CB	1:C:351:PHE:CD2	3.02	0.42
1:D:371:ASP:O	1:D:375:ILE:HG13	2.20	0.42
1:A:279:THR:HG22	4:A:812:HOH:O	2.19	0.42
1:B:212:GLU:O	1:B:216:LYS:HB2	2.20	0.42
1:D:293:ALA:O	1:D:295:PRO:HD3	2.20	0.42
1:D:364:LYS:HE3	4:D:835:HOH:O	2.19	0.42
1:A:313:VAL:HG13	1:A:314:TYR:H	1.84	0.42
1:D:247:LEU:HD23	1:D:268:ALA:HB1	2.02	0.42
1:D:401:GLN:C	1:D:403:GLY:N	2.76	0.42
1:B:213:ALA:HB1	1:B:293:ALA:CB	2.50	0.41
1:B:249:MET:O	1:B:252:LYS:HB3	2.20	0.41
1:C:465:ARG:C	1:C:467:MET:N	2.78	0.41
2:E:686:GLU:OE2	2:E:690:ARG:NH1	2.52	0.41
1:B:253:THR:O	1:B:254:LEU:C	2.62	0.41
1:C:243:ASP:OD1	1:C:245:GLU:HB3	2.21	0.41
1:B:255:VAL:HG12	1:B:257:LYS:N	2.34	0.41
1:B:255:VAL:CG1	1:B:258:LEU:HG	2.50	0.41
1:B:292:LYS:NZ	2:F:696:LYS:HG3	2.34	0.41
1:B:314:TYR:HB3	1:B:437:VAL:CG2	2.50	0.41
1:B:340:THR:HG22	1:B:342:GLU:N	2.35	0.41
1:C:236:ASN:OD1	1:C:236:ASN:C	2.62	0.41
1:C:445:GLN:O	1:C:446:ILE:HG13	2.19	0.41
1:D:255:VAL:O	1:D:257:LYS:N	2.49	0.41
2:E:684:GLY:CA	2:E:685:LEU:HD23	2.51	0.41
2:E:686:GLU:HA	2:E:689:ILE:HG12	2.02	0.41
2:G:689:ILE:HG12	2:G:690:ARG:N	2.34	0.41
1:A:313:VAL:HG13	1:A:314:TYR:N	2.35	0.41
1:B:247:LEU:HD23	1:B:343:PHE:HZ	1.84	0.41
1:B:278:CYS:C	1:B:280:SER:N	2.75	0.41
1:D:259:VAL:O	1:D:259:VAL:HG22	2.20	0.41
1:A:291:ALA:C	1:A:293:ALA:H	2.27	0.41
1:A:461:GLN:CG	1:A:464:TYR:CD2	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ILE:HG23	1:B:339:ILE:O	2.20	0.41
1:C:268:ALA:C	1:C:270:VAL:N	2.79	0.41
1:C:273:PHE:O	1:C:277:GLN:CG	2.64	0.41
1:C:282:GLU:OE1	1:C:282:GLU:CA	2.69	0.41
1:C:322:SER:HB3	1:C:366:ASN:HD21	1.85	0.41
1:D:280:SER:HB3	3:D:778:471:H4D2	2.03	0.41
1:D:288:THR:O	1:D:292:LYS:HG3	2.20	0.41
1:D:300:LEU:N	1:D:300:LEU:CD1	2.82	0.41
1:A:204:LYS:C	1:A:206:LEU:H	2.28	0.41
1:A:318:PHE:CE1	1:A:358:LYS:HE2	2.55	0.41
1:B:200:THR:O	1:B:204:LYS:CD	2.41	0.41
1:B:243:ASP:C	1:B:245:GLU:N	2.78	0.41
1:B:302:LEU:HD23	1:B:302:LEU:O	2.21	0.41
1:C:204:LYS:HA	1:C:204:LYS:HD2	1.78	0.41
1:C:394:VAL:O	1:C:394:VAL:HG13	2.20	0.41
1:A:226:ARG:NH2	1:A:325:MET:O	2.53	0.41
1:A:248:CYS:HG	1:A:271:ARG:HH22	1.61	0.41
1:C:459:LEU:O	1:C:462:GLU:O	2.39	0.41
1:D:332:VAL:O	1:D:333:ALA:C	2.61	0.41
2:E:693:LEU:HA	2:E:693:LEU:HD12	1.74	0.41
1:C:235:ASN:O	1:C:236:ASN:CB	2.69	0.41
1:D:264:GLN:H	1:D:264:GLN:HE21	1.67	0.41
1:A:326:ASN:OD1	1:A:326:ASN:C	2.64	0.41
1:B:246:THR:C	1:B:248:CYS:H	2.28	0.41
1:B:443:LEU:O	1:B:443:LEU:HG	2.20	0.41
1:C:358:LYS:NZ	1:C:440:HIS:CD2	2.89	0.41
1:C:423:PHE:N	1:C:424:PRO:HD2	2.36	0.41
1:D:247:LEU:O	1:D:251:GLU:CD	2.64	0.41
1:D:252:LYS:CA	1:D:258:LEU:HD13	2.50	0.41
1:B:263:ILE:HA	1:B:266:LYS:HE3	2.03	0.41
1:B:429:LYS:C	1:B:431:ALA:N	2.77	0.41
1:D:243:ASP:OD1	1:D:246:THR:HG23	2.21	0.41
1:A:210:ILE:HG21	1:A:377:LEU:HD23	2.03	0.40
1:A:214:TYR:C	1:A:216:LYS:H	2.29	0.40
1:B:265:ASN:O	1:B:265:ASN:OD1	2.38	0.40
1:C:254:LEU:HA	1:C:254:LEU:HD12	1.87	0.40
1:D:223:VAL:CG2	1:D:372:ASP:OD2	2.70	0.40
2:E:685:LEU:O	2:E:689:ILE:HG23	2.21	0.40
2:F:693:LEU:C	2:F:694:MET:HE2	2.46	0.40
1:A:274:HIS:O	1:A:275:CYS:C	2.63	0.40
1:A:302:LEU:CD1	2:E:693:LEU:HD23	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PHE:C	1:A:353:ASP:H	2.29	0.40
1:A:393:ASN:N	1:A:393:ASN:HD22	2.18	0.40
1:B:236:ASN:O	1:B:236:ASN:CG	2.63	0.40
1:B:401:GLN:C	1:B:403:GLY:N	2.78	0.40
1:C:396:HIS:HE1	4:C:785:HOH:O	2.04	0.40
1:B:212:GLU:OE1	2:F:700:TRP:CZ3	2.74	0.40
2:F:697:TYR:O	2:F:697:TYR:CD1	2.74	0.40
1:A:351:PHE:C	1:A:353:ASP:N	2.79	0.40
1:A:421:PHE:O	1:A:424:PRO:HD2	2.21	0.40
1:C:247:LEU:HD22	1:C:343:PHE:HZ	1.85	0.40
1:D:252:LYS:O	1:D:258:LEU:HD12	2.22	0.40
1:D:392:LEU:HB2	4:D:810:HOH:O	2.21	0.40
1:D:444:VAL:C	1:D:446:ILE:N	2.77	0.40
1:D:448:LYS:NZ	1:D:449:LYS:HG2	2.34	0.40
1:A:297:PHE:O	1:A:305:GLN:NE2	2.55	0.40
1:B:215:LEU:HD12	1:B:215:LEU:HA	1.87	0.40
1:C:291:ALA:C	1:C:293:ALA:H	2.29	0.40
1:C:311:TYR:CZ	1:C:389:PRO:HG2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/269 (99%)	205 (77%)	46 (17%)	16 (6%)	1	7
1	B	267/269 (99%)	222 (83%)	31 (12%)	14 (5%)	1	9
1	C	267/269 (99%)	198 (74%)	50 (19%)	19 (7%)	1	4
1	D	267/269 (99%)	214 (80%)	35 (13%)	18 (7%)	1	5
2	E	17/19 (90%)	9 (53%)	6 (35%)	2 (12%)	0	1
2	F	17/19 (90%)	11 (65%)	5 (29%)	1 (6%)	1	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	17/19 (90%)	14 (82%)	2 (12%)	1 (6%)	1	7
2	H	17/19 (90%)	14 (82%)	2 (12%)	1 (6%)	1	7
All	All	1136/1152 (99%)	887 (78%)	177 (16%)	72 (6%)	1	6

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	SER
1	A	256	ALA
1	A	346	SER
1	B	448	LYS
1	B	455	ALA
1	B	456	LEU
1	B	463	ILE
1	C	232	LYS
1	C	234	SER
1	C	269	GLU
1	C	394	VAL
1	D	260	ALA
1	D	349	LYS
1	D	352	CYS
1	D	455	ALA
2	E	683	MET
2	E	698	ASP
2	H	698	ASP
1	A	229	LEU
1	A	276	CYS
1	A	352	CYS
1	A	452	SER
1	A	462	GLU
1	A	465	ARG
1	A	466	ASP
1	B	234	SER
1	B	250	ALA
1	B	260	ALA
1	B	302	LEU
1	B	446	ILE
1	C	231	GLY
1	C	257	LYS
1	C	300	LEU
1	C	343	PHE

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Mol	Chain	Res	Type
1	C	447	ILE
1	D	231	GLY
1	D	295	PRO
1	D	394	VAL
1	D	446	ILE
1	D	462	GLU
1	D	463	ILE
2	F	695	GLY
1	A	201	ALA
1	A	265	ASN
1	A	300	LEU
1	A	394	VAL
1	B	232	LYS
1	B	244	MET
1	C	265	ASN
1	D	257	LYS
1	D	267	GLU
1	D	269	GLU
1	D	445	GLN
2	G	698	ASP
1	A	260	ALA
1	B	279	THR
1	C	446	ILE
1	C	466	ASP
1	D	223	VAL
1	D	268	ALA
1	D	279	THR
1	B	264	GLN
1	C	250	ALA
1	C	251	GLU
1	C	254	LEU
1	C	463	ILE
1	D	229	LEU
1	C	302	LEU
1	B	295	PRO
1	C	281	VAL
1	A	281	VAL
1	C	458	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	234/235 (100%)	183 (78%)	51 (22%)	1	6
1	B	234/235 (100%)	189 (81%)	45 (19%)	1	8
1	C	234/235 (100%)	197 (84%)	37 (16%)	2	13
1	D	234/235 (100%)	190 (81%)	44 (19%)	1	9
2	E	12/15 (80%)	4 (33%)	8 (67%)	0	0
2	F	13/15 (87%)	8 (62%)	5 (38%)	0	1
2	G	12/15 (80%)	7 (58%)	5 (42%)	0	0
2	H	12/15 (80%)	9 (75%)	3 (25%)	0	3
All	All	985/1000 (98%)	787 (80%)	198 (20%)	1	7

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	ASP
1	A	204	LYS
1	A	223	VAL
1	A	227	VAL
1	A	230	SER
1	A	232	LYS
1	A	235	ASN
1	A	251	GLU
1	A	253	THR
1	A	254	LEU
1	A	258	LEU
1	A	259	VAL
1	A	263	ILE
1	A	264	GLN
1	A	265	ASN
1	A	269	GLU
1	A	271	ARG
1	A	273	PHE
1	A	280	SER

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Mol	Chain	Res	Type
1	A	283	THR
1	A	300	LEU
1	A	301	ASP
1	A	302	LEU
1	A	304	ASP
1	A	321	LEU
1	A	334	TYR
1	A	353	ASP
1	A	355	MET
1	A	361	PHE
1	A	363	MET
1	A	371	ASP
1	A	373	SER
1	A	382	ILE
1	A	383	ILE
1	A	387	ASP
1	A	392	LEU
1	A	396	HIS
1	A	410	LEU
1	A	415	ASN
1	A	420	ILE
1	A	428	GLN
1	A	435	GLN
1	A	438	THR
1	A	444	VAL
1	A	448	LYS
1	A	453	ASP
1	A	456	LEU
1	A	459	LEU
1	A	460	LEU
1	A	461	GLN
1	A	463	ILE
1	B	206	LEU
1	B	215	LEU
1	B	216	LYS
1	B	220	MET
1	B	227	VAL
1	B	232	LYS
1	B	244	MET
1	B	247	LEU
1	B	248	CYS
1	B	251	GLU

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Mol	Chain	Res	Type
1	B	266	LYS
1	B	269	GLU
1	B	282	GLU
1	B	286	GLU
1	B	287	LEU
1	B	295	PRO
1	B	302	LEU
1	B	303	ASN
1	B	322	SER
1	B	324	VAL
1	B	334	TYR
1	B	350	PRO
1	B	353	ASP
1	B	358	LYS
1	B	363	MET
1	B	377	LEU
1	B	392	LEU
1	B	394	VAL
1	B	407	VAL
1	B	408	LEU
1	B	412	LEU
1	B	420	ILE
1	B	422	LEU
1	B	435	GLN
1	B	436	LEU
1	B	437	VAL
1	B	442	GLN
1	B	444	VAL
1	B	445	GLN
1	B	446	ILE
1	B	450	THR
1	B	453	ASP
1	B	456	LEU
1	B	459	LEU
1	B	460	LEU
1	C	208	LYS
1	C	209	ARG
1	C	226	ARG
1	C	230	SER
1	C	232	LYS
1	C	236	ASN
1	C	251	GLU

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Mol	Chain	Res	Type
1	C	254	LEU
1	C	259	VAL
1	C	261	ASN
1	C	264	GLN
1	C	267	GLU
1	C	269	GLU
1	C	282	GLU
1	C	302	LEU
1	C	303	ASN
1	C	310	LYS
1	C	340	THR
1	C	345	LYS
1	C	349	LYS
1	C	363	MET
1	C	382	ILE
1	C	394	VAL
1	C	396	HIS
1	C	401	GLN
1	C	412	LEU
1	C	415	ASN
1	C	420	ILE
1	C	438	THR
1	C	452	SER
1	C	456	LEU
1	C	459	LEU
1	C	460	LEU
1	C	461	GLN
1	C	462	GLU
1	C	463	ILE
1	C	465	ARG
1	D	208	LYS
1	D	209	ARG
1	D	223	VAL
1	D	230	SER
1	D	251	GLU
1	D	253	THR
1	D	254	LEU
1	D	258	LEU
1	D	263	ILE
1	D	264	GLN
1	D	267	GLU
1	D	269	GLU

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Mol	Chain	Res	Type
1	D	271	ARG
1	D	276	CYS
1	D	282	GLU
1	D	300	LEU
1	D	301	ASP
1	D	303	ASN
1	D	313	VAL
1	D	327	LYS
1	D	346	SER
1	D	350	PRO
1	D	352	CYS
1	D	382	ILE
1	D	391	LEU
1	D	392	LEU
1	D	394	VAL
1	D	399	LYS
1	D	405	VAL
1	D	407	VAL
1	D	409	ARG
1	D	414	SER
1	D	420	ILE
1	D	430	MET
1	D	438	THR
1	D	443	LEU
1	D	445	GLN
1	D	447	ILE
1	D	453	ASP
1	D	456	LEU
1	D	459	LEU
1	D	461	GLN
1	D	465	ARG
1	D	468	TYR
2	E	683	MET
2	E	685	LEU
2	E	688	ILE
2	E	689	ILE
2	E	693	LEU
2	E	694	MET
2	E	697	TYR
2	E	700	TRP
2	F	685	LEU
2	F	689	ILE

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Mol	Chain	Res	Type
2	F	693	LEU
2	F	694	MET
2	F	697	TYR
2	G	688	ILE
2	G	689	ILE
2	G	691	LYS
2	G	693	LEU
2	G	700	TRP
2	H	686	GLU
2	H	689	ILE
2	H	693	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	261	ASN
1	A	264	GLN
1	A	277	GLN
1	A	299	ASN
1	A	305	GLN
1	A	366	ASN
1	A	406	HIS
1	A	411	HIS
1	A	413	GLN
1	A	415	ASN
1	A	416	HIS
1	A	442	GLN
1	B	217	ASN
1	B	242	HIS
1	B	261	ASN
1	B	264	GLN
1	B	277	GLN
1	B	336	ASN
1	B	406	HIS
1	B	411	HIS
1	B	416	HIS
1	B	445	GLN
1	C	236	ASN
1	C	242	HIS
1	C	264	GLN
1	C	299	ASN

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Mol	Chain	Res	Type
1	C	303	ASN
1	C	336	ASN
1	C	366	ASN
1	C	393	ASN
1	C	401	GLN
1	C	415	ASN
1	C	440	HIS
1	C	445	GLN
1	C	461	GLN
1	D	219	ASN
1	D	235	ASN
1	D	242	HIS
1	D	264	GLN
1	D	299	ASN
1	D	303	ASN
1	D	336	ASN
1	D	366	ASN
1	D	393	ASN
1	D	401	GLN
1	D	416	HIS
1	D	445	GLN
1	D	457	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
3	471	A	775	-	47,48,48	2.40	22 (46%)	62,66,66	1.75	10 (16%)
3	471	D	778	-	47,48,48	2.39	22 (46%)	62,66,66	1.94	10 (16%)
3	471	C	777	-	47,48,48	2.42	22 (46%)	62,66,66	1.86	11 (17%)
3	471	B	776	-	47,48,48	2.41	22 (46%)	62,66,66	2.08	12 (19%)

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
3	471	A	775	-	-	9/39/39/39	0/4/4/4
3	471	D	778	-	-	6/39/39/39	0/4/4/4
3	471	C	777	-	-	9/39/39/39	0/4/4/4
3	471	B	776	-	-	10/39/39/39	0/4/4/4

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	777	471	C3I-C3G	-6.37	1.34	1.47
3	A	775	471	C3I-C3G	-6.36	1.34	1.47
3	C	777	471	C1H-C1G	-6.34	1.40	1.49
3	B	776	471	C3I-C3G	-6.33	1.34	1.47
3	D	778	471	C3I-C3G	-6.32	1.34	1.47
3	B	776	471	C1H-C1G	-6.22	1.40	1.49
3	C	777	471	C3G-N3H	6.00	1.38	1.30
3	A	775	471	C3G-N3H	5.96	1.38	1.30
3	D	778	471	C3G-N3H	5.95	1.38	1.30
3	A	775	471	C1H-C1G	-5.93	1.40	1.49
3	D	778	471	C1H-C1G	-5.93	1.40	1.49
3	B	776	471	C3G-N3H	5.92	1.38	1.30
3	B	776	471	C1A-N	4.47	1.39	1.33
3	C	777	471	C1A-N	4.47	1.39	1.33
3	A	775	471	C1A-N	4.43	1.39	1.33
3	D	778	471	C1A-N	4.40	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	775	471	C1M-C1H	-3.23	1.34	1.39
3	C	777	471	C1M-C1H	-3.22	1.34	1.39
3	B	776	471	C3N-C3I	-3.21	1.34	1.39
3	D	778	471	C1M-C1H	-3.21	1.34	1.39
3	A	775	471	C1I-C1H	-3.20	1.34	1.39
3	D	778	471	C3N-C3I	-3.19	1.34	1.39
3	C	777	471	C3J-C3I	-3.18	1.34	1.39
3	B	776	471	C3J-C3I	-3.16	1.34	1.39
3	B	776	471	C1M-C1H	-3.16	1.34	1.39
3	D	778	471	C3J-C3I	-3.16	1.34	1.39
3	A	775	471	C3J-C3I	-3.15	1.34	1.39
3	C	777	471	C1I-C1H	-3.14	1.34	1.39
3	A	775	471	C3N-C3I	-3.14	1.34	1.39
3	B	776	471	C1I-C1H	-3.14	1.34	1.39
3	C	777	471	C3N-C3I	-3.13	1.34	1.39
3	D	778	471	C1I-C1H	-3.10	1.34	1.39
3	B	776	471	C1L-C1K	-2.87	1.34	1.39
3	A	775	471	C1L-C1K	-2.86	1.34	1.39
3	C	777	471	C1J-C1K	-2.84	1.34	1.39
3	D	778	471	C1J-C1K	-2.84	1.34	1.39
3	C	777	471	C1L-C1K	-2.82	1.34	1.39
3	B	776	471	C1J-C1K	-2.82	1.34	1.39
3	D	778	471	C1L-C1K	-2.82	1.34	1.39
3	A	775	471	C1J-C1K	-2.81	1.34	1.39
3	B	776	471	CE1-CD1	-2.68	1.34	1.38
3	C	777	471	C1J-C1I	-2.66	1.34	1.38
3	A	775	471	CE2-CD2	-2.64	1.34	1.38
3	D	778	471	C1J-C1I	-2.63	1.34	1.38
3	A	775	471	C1J-C1I	-2.62	1.34	1.38
3	A	775	471	CE1-CD1	-2.62	1.34	1.38
3	D	778	471	C1M-C1L	-2.61	1.34	1.38
3	C	777	471	C1M-C1L	-2.61	1.34	1.38
3	C	777	471	CE2-CD2	-2.61	1.34	1.38
3	C	777	471	CE1-CD1	-2.60	1.34	1.38
3	D	778	471	CE1-CD1	-2.60	1.34	1.38
3	B	776	471	C1M-C1L	-2.60	1.34	1.38
3	B	776	471	CE2-CD2	-2.60	1.34	1.38
3	B	776	471	C1J-C1I	-2.59	1.34	1.38
3	A	775	471	C1M-C1L	-2.58	1.34	1.38
3	D	778	471	CE2-CD2	-2.58	1.34	1.38
3	B	776	471	C3K-C3J	-2.56	1.34	1.38
3	A	775	471	C3K-C3J	-2.56	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	778	471	C3M-C3N	-2.54	1.34	1.38
3	D	778	471	C3K-C3J	-2.53	1.34	1.38
3	B	776	471	C3M-C3N	-2.53	1.34	1.38
3	C	777	471	C3M-C3N	-2.51	1.34	1.38
3	C	777	471	C1F-C1A	-2.51	1.33	1.38
3	C	777	471	C3K-C3J	-2.50	1.34	1.38
3	B	776	471	C1F-C1A	-2.48	1.33	1.38
3	A	775	471	C1F-C1A	-2.48	1.33	1.38
3	D	778	471	C1F-C1A	-2.48	1.33	1.38
3	A	775	471	C3M-C3N	-2.47	1.34	1.38
3	D	778	471	CE2-CZ	-2.24	1.34	1.38
3	A	775	471	CE1-CZ	-2.23	1.34	1.38
3	D	778	471	CD1-CG	-2.23	1.34	1.38
3	C	777	471	CD1-CG	-2.22	1.34	1.38
3	B	776	471	CE2-CZ	-2.21	1.34	1.38
3	C	777	471	CE2-CZ	-2.21	1.34	1.38
3	B	776	471	C1F-C1G	2.20	1.50	1.43
3	B	776	471	CE1-CZ	-2.20	1.34	1.38
3	A	775	471	CD1-CG	-2.20	1.34	1.38
3	B	776	471	CD2-CG	-2.20	1.34	1.38
3	A	775	471	CD2-CG	-2.20	1.34	1.38
3	D	778	471	CE1-CZ	-2.19	1.34	1.38
3	D	778	471	C1F-C1G	2.19	1.50	1.43
3	C	777	471	C1F-C1G	2.18	1.50	1.43
3	C	777	471	CE1-CZ	-2.18	1.34	1.38
3	A	775	471	C1F-C1G	2.18	1.50	1.43
3	C	777	471	CD2-CG	-2.17	1.34	1.38
3	A	775	471	CE2-CZ	-2.17	1.34	1.38
3	D	778	471	CD2-CG	-2.15	1.34	1.38
3	B	776	471	CD1-CG	-2.13	1.34	1.38

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	776	471	C3E-C3D-C3C	-6.94	129.54	135.22
3	D	778	471	C3E-C3D-C3C	-6.79	129.67	135.22
3	A	775	471	C3E-C3D-C3C	-6.64	129.78	135.22
3	C	777	471	C3E-C3D-C3C	-6.59	129.83	135.22
3	D	778	471	C4A-CA-N	5.98	121.89	108.97
3	B	776	471	C4A-CA-N	5.95	121.82	108.97
3	C	777	471	O3F-C3G-N3H	-5.41	108.47	114.37
3	B	776	471	C1B-C1A-N	5.28	125.31	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	776	471	O3F-C3G-N3H	-5.12	108.77	114.37
3	B	776	471	C1F-C1A-N	-5.07	117.31	121.29
3	D	778	471	O3F-C3D-C3E	5.04	122.48	115.88
3	A	775	471	O3F-C3G-N3H	-4.99	108.92	114.37
3	B	776	471	O3F-C3D-C3E	4.91	122.30	115.88
3	D	778	471	O3F-C3G-N3H	-4.87	109.06	114.37
3	C	777	471	O3F-C3D-C3E	4.86	122.24	115.88
3	A	775	471	O3F-C3D-C3E	4.78	122.14	115.88
3	D	778	471	C1B-C1A-N	4.47	124.30	118.75
3	D	778	471	C1A-C1F-C1G	4.25	133.35	124.20
3	C	777	471	C1B-C1A-N	4.24	124.01	118.75
3	A	775	471	C1B-C1A-N	4.10	123.84	118.75
3	C	777	471	C4A-CA-N	3.23	115.94	108.97
3	C	777	471	C4A-CA-CB	3.22	119.54	110.37
3	B	776	471	O3F-C3G-C3I	3.00	123.95	118.73
3	B	776	471	C1H-C1G-C1F	2.90	126.02	119.83
3	C	777	471	C1A-C1F-C1G	2.89	130.43	124.20
3	A	775	471	C1A-C1F-C1G	2.86	130.36	124.20
3	B	776	471	C4A-CA-CB	2.85	118.50	110.37
3	A	775	471	OH-C3A-C3B	2.82	113.96	107.28
3	B	776	471	OH-C3A-C3B	2.80	113.90	107.28
3	A	775	471	CG-CB-CA	2.79	119.84	113.71
3	C	777	471	OH-C3A-C3B	2.79	113.87	107.28
3	D	778	471	O3F-C3G-C3I	2.76	123.54	118.73
3	D	778	471	C4A-CA-CB	2.76	118.23	110.37
3	C	777	471	O3F-C3G-C3I	2.66	123.37	118.73
3	A	775	471	O3F-C3G-C3I	2.50	123.09	118.73
3	B	776	471	O1G-C1G-C1H	-2.47	115.30	119.20
3	A	775	471	C1F-C1A-N	-2.38	119.42	121.29
3	B	776	471	C1A-C1F-C1G	2.36	129.28	124.20
3	A	775	471	C1H-C1G-C1F	2.28	124.71	119.83
3	D	778	471	C1B-C1A-C1F	-2.27	115.55	120.13
3	D	778	471	OH-C3A-C3B	2.24	112.57	107.28
3	C	777	471	C1B-C1A-C1F	-2.07	115.96	120.13
3	C	777	471	C4A-N4B-C4C	2.02	127.03	122.69

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	776	471	C4A-CA-N-C1A
3	B	776	471	N4B-C4A-CA-N

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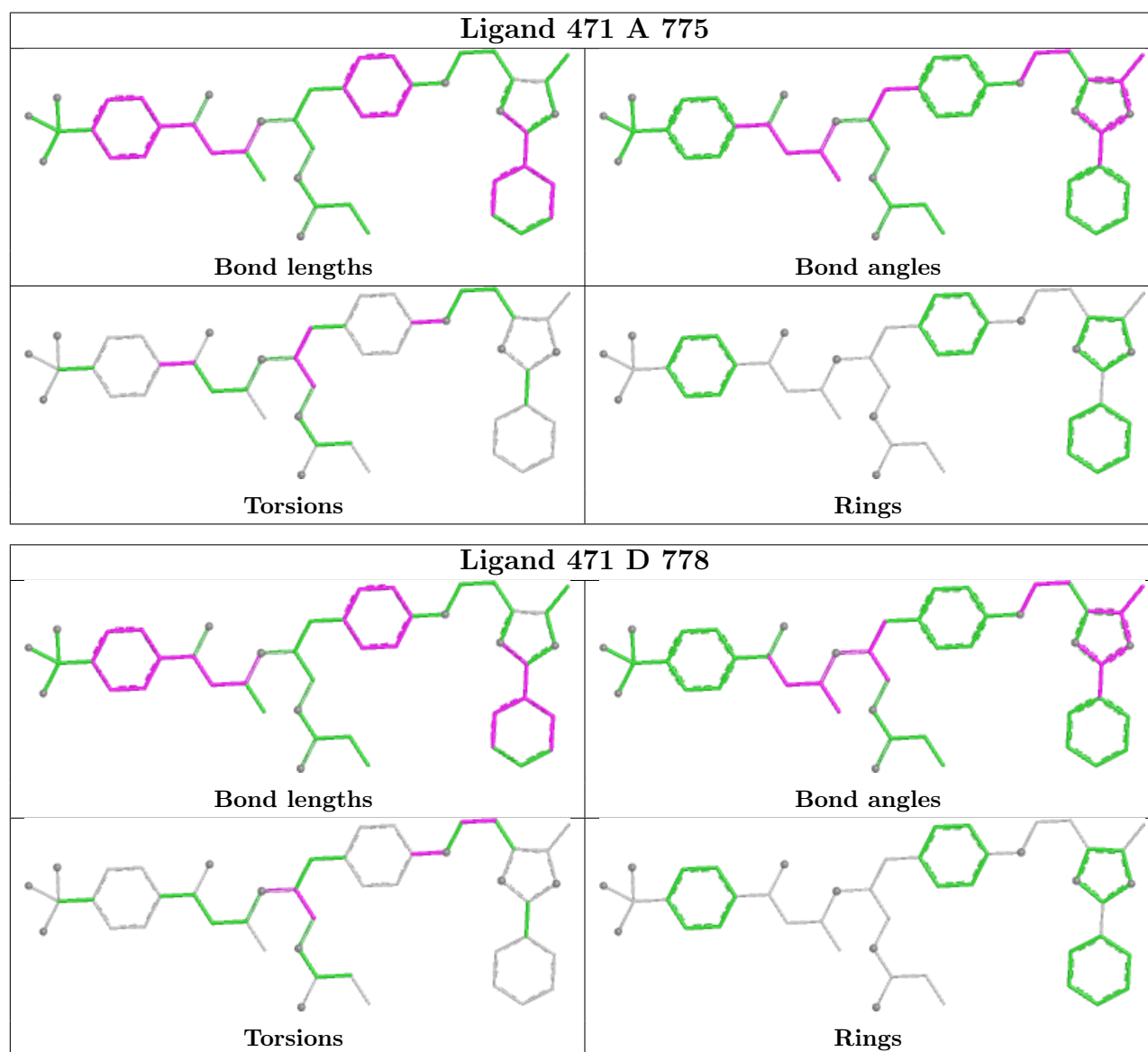
Mol	Chain	Res	Type	Atoms
3	C	777	471	N4B-C4A-CA-N
3	C	777	471	C1F-C1G-C1H-C1I
3	C	777	471	O1G-C1G-C1H-C1I
3	C	777	471	OH-C3A-C3B-C3C
3	D	778	471	C4A-CA-N-C1A
3	D	778	471	N4B-C4A-CA-N
3	C	777	471	O1G-C1G-C1H-C1M
3	C	777	471	C1F-C1G-C1H-C1M
3	B	776	471	O1G-C1G-C1H-C1M
3	A	775	471	N4B-C4A-CA-N
3	B	776	471	C1F-C1G-C1H-C1M
3	B	776	471	O1G-C1G-C1H-C1I
3	B	776	471	C1F-C1G-C1H-C1I
3	C	777	471	CE1-CZ-OH-C3A
3	A	775	471	CE1-CZ-OH-C3A
3	A	775	471	CE2-CZ-OH-C3A
3	B	776	471	CE1-CZ-OH-C3A
3	C	777	471	CE2-CZ-OH-C3A
3	D	778	471	CE1-CZ-OH-C3A
3	B	776	471	CE2-CZ-OH-C3A
3	D	778	471	CE2-CZ-OH-C3A
3	A	775	471	N4B-C4A-CA-CB
3	B	776	471	N4B-C4A-CA-CB
3	C	777	471	N4B-C4A-CA-CB
3	D	778	471	N4B-C4A-CA-CB
3	A	775	471	N-CA-CB-CG
3	A	775	471	O1G-C1G-C1H-C1M
3	A	775	471	O1G-C1G-C1H-C1I
3	A	775	471	C1F-C1G-C1H-C1M
3	A	775	471	C1F-C1G-C1H-C1I
3	D	778	471	OH-C3A-C3B-C3C
3	B	776	471	CA-C4A-N4B-C4C

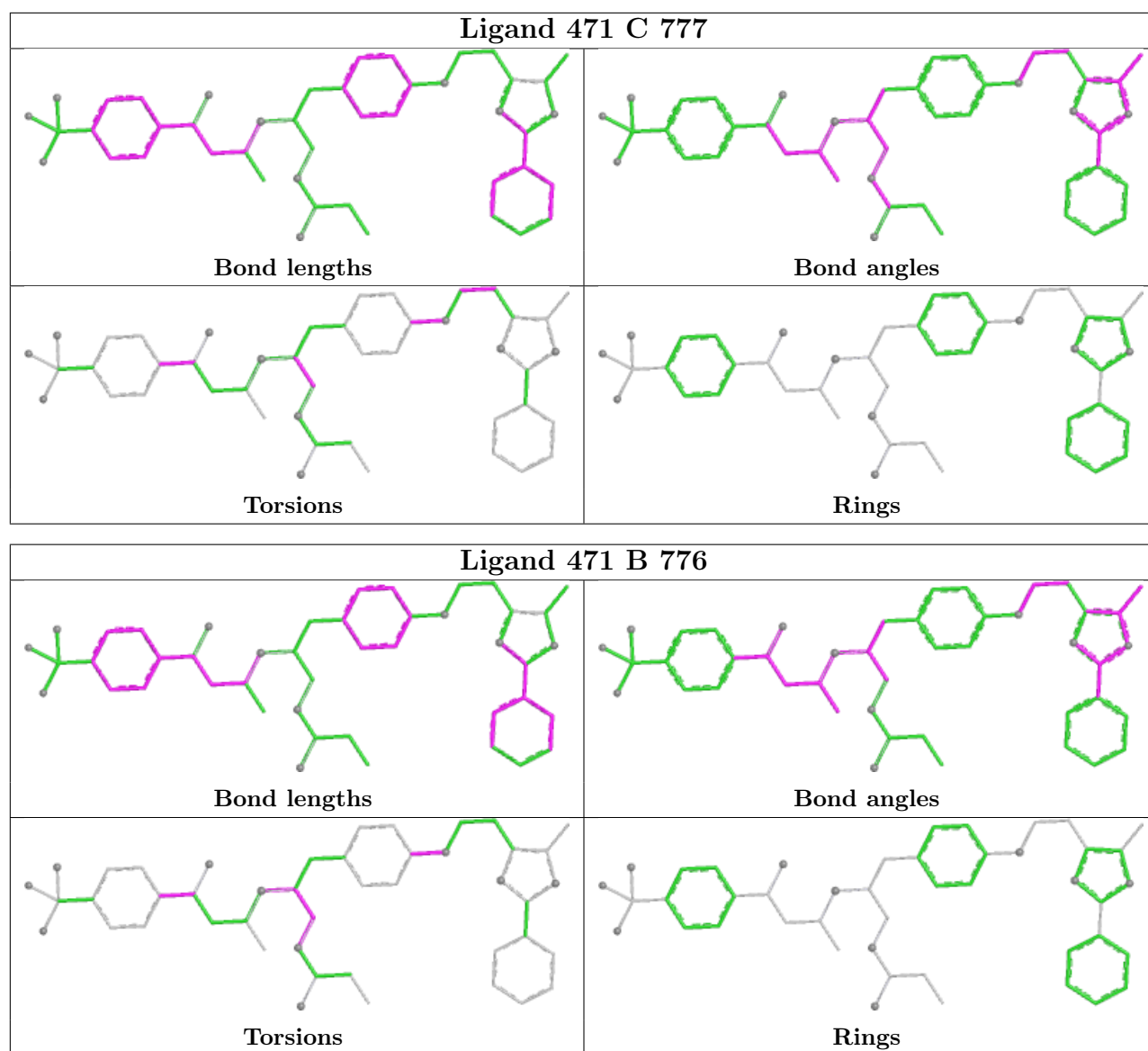
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	775	471	1	0
3	D	778	471	3	0
3	C	777	471	2	0
3	B	776	471	8	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.