



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:06 AM UTC

PDB ID : 1IB1 / pdb_00001ib1
Title : CRYSTAL STRUCTURE OF THE 14-3-3 ZETA:SEROTONIN N-ACETYLTRANSFERASE COMPLEX
Authors : Obsil, T.; Ghirlando, R.; Klein, D.C.; Ganguly, S.; Dyda, F.
Deposited on : 2001-03-26
Resolution : 2.70 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

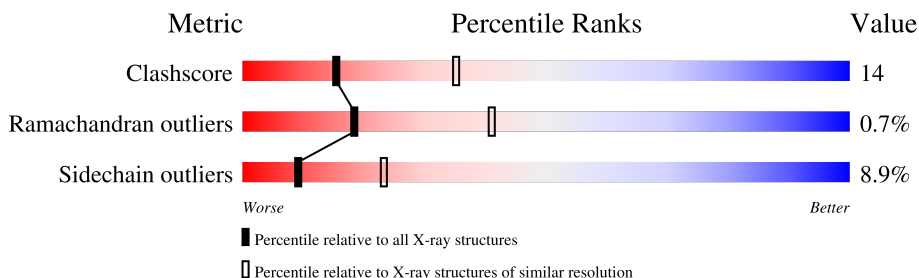
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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	245	58% 30% . . 7%
1	B	245	62% 28% . 7%
1	C	245	61% 27% . 7%
1	D	245	60% 29% . 7%
2	E	200	62% 24% . 10%
2	F	200	58% 28% . 10%
2	G	200	60% 26% . 10%
2	H	200	64% 22% . 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13407 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 14-3-3 ZETA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1821	1142	306	364	9			
1	B	227	Total	C	N	O	S	0	0	0
			1821	1142	306	364	9			
1	C	227	Total	C	N	O	S	0	0	0
			1821	1142	306	364	9			
1	D	227	Total	C	N	O	S	0	0	0
			1821	1142	306	364	9			

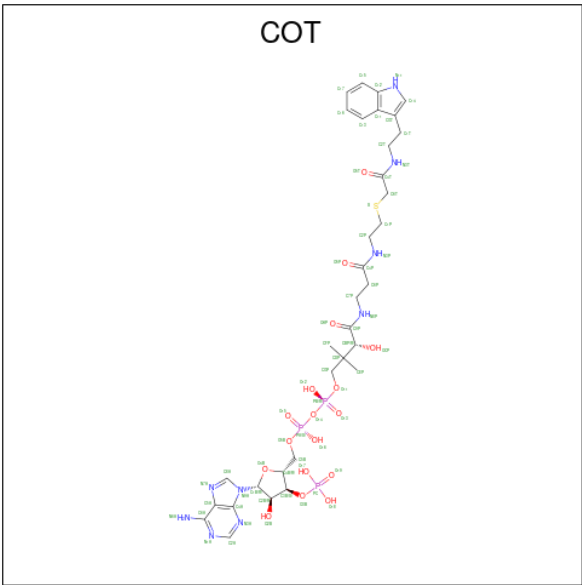
- Molecule 2 is a protein called SEROTONIN N-ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
2	E	179	Total 1415	C 897	N 263	O 246	P 1	S 8	0	0	0
2	F	179	Total 1415	C 897	N 263	O 246	P 1	S 8	0	0	0
2	G	179	Total 1415	C 897	N 263	O 246	P 1	S 8	0	0	0
2	H	179	Total 1415	C 897	N 263	O 246	P 1	S 8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	31	TPO	THR	modified residue	UNP Q29495
F	31	TPO	THR	modified residue	UNP Q29495
G	31	TPO	THR	modified residue	UNP Q29495
H	31	TPO	THR	modified residue	UNP Q29495

- Molecule 3 is COA-S-ACETYL TRYPTAMINE (CCD ID: COT) (formula: $C_{33}H_{48}N_9O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	E	1	Total	C	N	O	P	S	0	0
			63	33	9	17	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			63	33	9	17	3	1		
3	G	1	Total	C	N	O	P	S	0	0
			63	33	9	17	3	1		
3	H	1	Total	C	N	O	P	S	0	0
			63	33	9	17	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	20	Total	O	0	0
			20	20		
4	C	42	Total	O	0	0
			42	42		
4	D	31	Total	O	0	0
			31	31		
4	E	24	Total	O	0	0
			24	24		
4	F	21	Total	O	0	0
			21	21		
4	G	23	Total	O	0	0
			23	23		
4	H	22	Total	O	0	0
			22	22		

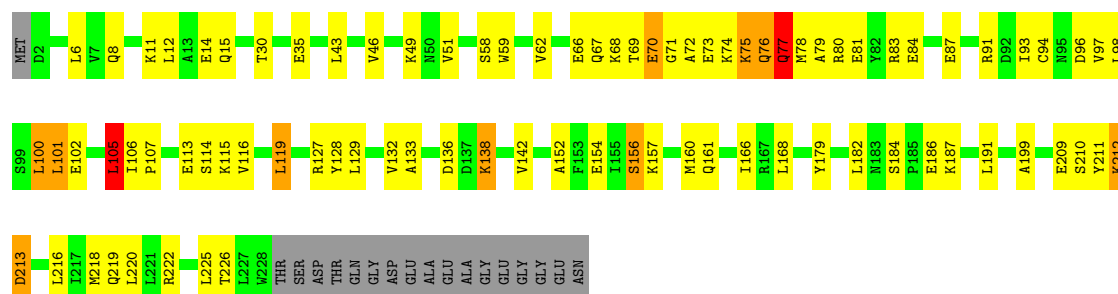
3 Residue-property plots

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: 14-3-3 ZETA ISOFORM

Chain A: 



• Molecule 1: 14-3-3 ZETA ISOFORM

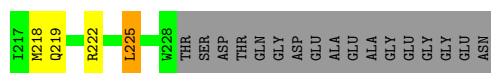
Chain B: 



• Molecule 1: 14-3-3 ZETA ISOFORM

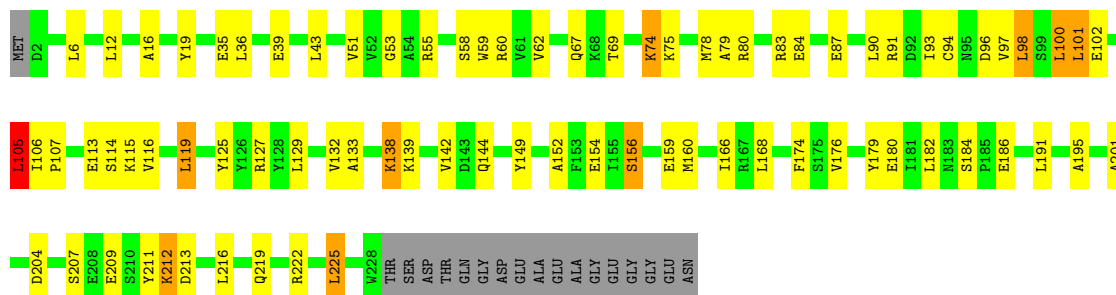
Chain C: 





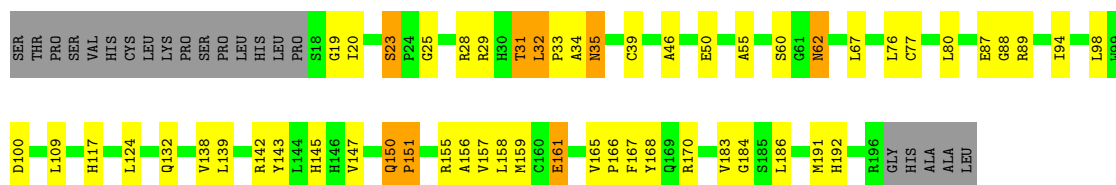
• Molecule 1: 14-3-3 ZETA ISOFORM

Chain D: 60% 29% 7%



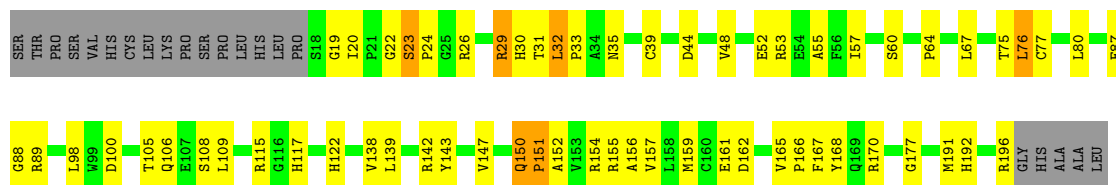
• Molecule 2: SEROTONIN N-ACETYLTRANSFERASE

Chain E: 62% 24% 10%



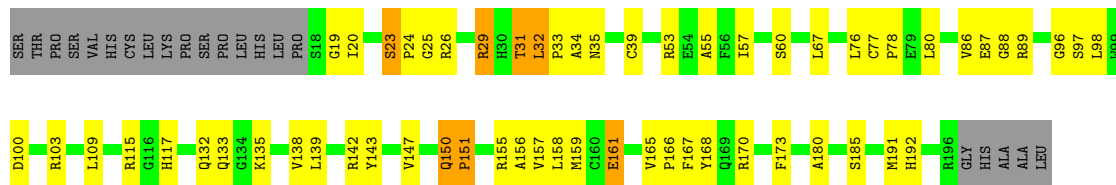
• Molecule 2: SEROTONIN N-ACETYLTRANSFERASE

Chain F: 58% 28% 10%



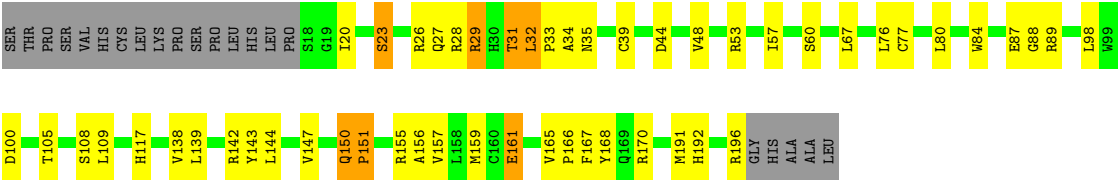
• Molecule 2: SEROTONIN N-ACETYLTRANSFERASE

Chain G: 60% 26% 10%



• Molecule 2: SEROTONIN N-ACETYLTRANSFERASE

Chain H: 64% 22% 10%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.72Å 75.08Å 101.78Å 90.14° 90.06° 63.04°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	99.3 (20.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.204 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13407	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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: COT, TPO

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	0.50	0/1846	1.10	13/2482 (0.5%)
1	B	0.49	0/1846	0.99	5/2482 (0.2%)
1	C	0.50	0/1846	1.00	5/2482 (0.2%)
1	D	0.48	0/1846	1.02	7/2482 (0.3%)
2	E	0.50	0/1443	1.06	7/1956 (0.4%)
2	F	0.51	0/1443	1.10	10/1956 (0.5%)
2	G	0.50	0/1443	1.05	7/1956 (0.4%)
2	H	0.50	0/1443	1.05	5/1956 (0.3%)
All	All	0.50	0/13156	1.05	59/17752 (0.3%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	TYR	N-CA-C	11.53	123.83	111.03
2	H	150	GLN	CA-C-N	10.25	132.65	119.84
2	H	150	GLN	C-N-CA	10.25	132.65	119.84
1	A	76	GLN	OE1-CD-NE2	-10.18	112.42	122.60
1	A	77	GLN	OE1-CD-NE2	-9.74	112.86	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	150	GLN	CA-C-N	9.71	131.98	119.84
2	E	150	GLN	C-N-CA	9.71	131.98	119.84
2	F	106	GLN	OE1-CD-NE2	-9.54	113.06	122.60
2	G	150	GLN	CA-C-N	9.45	131.66	119.84
2	G	150	GLN	C-N-CA	9.45	131.66	119.84
2	F	150	GLN	CA-C-N	9.10	131.21	119.84
2	F	150	GLN	C-N-CA	9.10	131.21	119.84
2	F	55	ALA	N-CA-C	9.01	121.09	111.28
2	F	23	SER	CA-C-N	8.60	128.18	119.24
2	F	23	SER	C-N-CA	8.60	128.18	119.24
2	E	23	SER	CA-C-N	8.20	127.76	119.24
2	E	23	SER	C-N-CA	8.20	127.76	119.24
2	H	23	SER	CA-C-N	8.16	127.73	119.24
2	H	23	SER	C-N-CA	8.16	127.73	119.24
2	G	23	SER	CA-C-N	7.64	127.19	119.24
2	G	23	SER	C-N-CA	7.64	127.19	119.24
1	C	105	LEU	N-CA-C	7.36	119.00	110.97
2	E	55	ALA	N-CA-C	7.33	120.14	111.71
1	A	77	GLN	CG-CD-NE2	6.98	126.87	116.40
1	B	105	LEU	N-CA-C	6.87	118.46	110.97
2	F	106	GLN	CG-CD-NE2	6.77	126.56	116.40
1	D	105	LEU	N-CA-C	6.67	118.24	110.97
1	A	138	LYS	N-CA-C	6.67	118.20	111.07
2	G	55	ALA	N-CA-C	6.59	118.26	111.14
1	A	105	LEU	N-CA-C	6.59	118.15	110.97
1	A	76	GLN	CG-CD-NE2	6.45	126.07	116.40
2	F	39	CYS	N-CA-C	-6.16	100.47	110.20
1	B	211	TYR	N-CA-C	6.12	123.84	110.80
1	A	213	ASP	N-CA-C	-6.00	106.09	113.41
1	D	138	LYS	N-CA-C	5.85	117.33	111.07
2	E	39	CYS	N-CA-C	-5.76	101.10	110.20
1	D	179	TYR	N-CA-C	5.64	117.10	111.07
2	G	39	CYS	N-CA-C	-5.62	101.32	110.20
2	H	39	CYS	N-CA-C	-5.54	101.45	110.20
1	D	133	ALA	N-CA-C	5.51	118.34	110.24
2	G	19	GLY	N-CA-C	5.44	126.06	113.18
2	F	162	ASP	N-CA-C	5.44	117.91	111.33
2	F	19	GLY	N-CA-C	5.43	126.05	113.18
2	E	19	GLY	N-CA-C	5.41	125.99	113.18
1	C	211	TYR	N-CA-C	5.37	119.77	112.04
1	C	179	TYR	N-CA-C	5.36	116.93	111.14
1	A	179	TYR	N-CA-C	5.33	116.78	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	SER	CA-C-N	5.25	124.70	119.24
1	D	184	SER	C-N-CA	5.25	124.70	119.24
1	B	19	TYR	N-CA-C	5.19	117.67	111.71
1	A	76	GLN	N-CA-C	-5.17	105.72	112.23
1	B	179	TYR	N-CA-C	5.14	116.70	111.14
1	A	184	SER	CA-C-N	5.08	124.53	119.24
1	A	184	SER	C-N-CA	5.08	124.53	119.24
1	D	159	GLU	N-CA-C	5.08	120.11	113.30
1	B	138	LYS	N-CA-C	5.06	117.20	111.02
1	A	136	ASP	N-CA-C	5.03	117.65	111.82
1	C	184	SER	CA-C-N	5.00	124.44	119.24
1	C	184	SER	C-N-CA	5.00	124.44	119.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	125	TYR	Sidechain
1	C	125	TYR	Sidechain
1	D	125	TYR	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1821	0	1809	72	0
1	B	1821	0	1809	45	1
1	C	1821	0	1809	53	0
1	D	1821	0	1809	57	0
2	E	1415	0	1382	37	0
2	F	1415	0	1382	45	1
2	G	1415	0	1382	48	0
2	H	1415	0	1382	37	0
3	E	63	0	44	1	0
3	F	63	0	44	1	0
3	G	63	0	44	1	0
3	H	63	0	44	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	28	0	0	19	0
4	B	20	0	0	6	0
4	C	42	0	0	7	1
4	D	31	0	0	13	1
4	E	24	0	0	2	0
4	F	21	0	0	6	0
4	G	23	0	0	11	0
4	H	22	0	0	2	0
All	All	13407	0	12940	353	2

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 14.

All (353) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:ARG:HD2	4:D:3635:HOH:O	1.34	1.22
1:D:144:GLN:HG3	4:D:4412:HOH:O	1.37	1.20
1:A:73:GLU:HB2	4:A:2487:HOH:O	1.57	1.03
1:A:75:LYS:HE3	1:B:8:GLN:HG2	1.48	0.94
2:E:159:MET:HE2	4:E:3297:HOH:O	1.70	0.92
1:A:226:THR:CB	4:A:3511:HOH:O	2.24	0.86
1:C:74:LYS:HD3	1:C:74:LYS:N	1.90	0.84
1:A:226:THR:HB	4:A:3511:HOH:O	1.77	0.83
1:A:75:LYS:CE	1:B:8:GLN:HG2	2.10	0.81
1:A:116:VAL:HG11	1:A:160:MET:HE1	1.63	0.81
1:D:116:VAL:HG11	1:D:160:MET:HE1	1.61	0.81
1:B:116:VAL:HG11	1:B:160:MET:HE1	1.64	0.78
1:C:129:LEU:HD21	4:C:2870:HOH:O	1.83	0.77
1:A:73:GLU:CB	4:A:2487:HOH:O	2.22	0.77
2:F:117:HIS:HB3	4:F:3100:HOH:O	1.85	0.76
1:C:78:MET:HB3	4:C:3675:HOH:O	1.86	0.75
2:F:76:LEU:HG	2:G:185:SER:HA	1.69	0.75
2:F:154:ARG:NH1	4:F:3100:HOH:O	2.18	0.74
1:C:116:VAL:HG11	1:C:160:MET:HE1	1.70	0.72
2:G:115:ARG:HD2	4:G:3362:HOH:O	1.89	0.72
1:C:69:THR:HB	1:C:76:GLN:HG2	1.72	0.72
1:A:73:GLU:CA	4:A:2487:HOH:O	2.36	0.71
2:G:115:ARG:NH1	4:G:3483:HOH:O	2.23	0.70
1:B:156:SER:HA	1:B:160:MET:HE3	1.73	0.70
1:C:156:SER:HA	1:C:160:MET:HE3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:115:ARG:CD	4:G:3362:HOH:O	2.40	0.69
1:C:211:TYR:O	1:C:212:LYS:HG2	1.93	0.69
1:A:210:SER:HB2	1:A:212:LYS:NZ	2.09	0.68
1:B:210:SER:O	1:B:212:LYS:HG3	1.93	0.68
1:D:19:TYR:HD2	4:D:3597:HOH:O	1.77	0.68
1:A:74:LYS:C	1:A:76:GLN:H	2.02	0.67
2:G:96:GLY:O	4:G:2928:HOH:O	2.13	0.67
1:A:66:GLU:O	1:A:76:GLN:NE2	2.27	0.66
2:G:168:TYR:HB2	2:G:191:MET:HE2	1.75	0.66
1:A:119:LEU:HB3	1:A:152:ALA:HB2	1.77	0.66
1:A:75:LYS:HE3	1:B:8:GLN:CG	2.24	0.65
1:A:51:VAL:HG12	1:A:93:ILE:HD13	1.78	0.65
2:E:168:TYR:HB2	2:E:191:MET:HE2	1.77	0.64
1:D:139:LYS:HB2	4:D:4357:HOH:O	1.96	0.64
2:F:32:LEU:HD22	2:F:33:PRO:HD2	1.80	0.64
1:C:77:GLN:O	1:C:81:GLU:HG3	1.98	0.64
1:D:60:ARG:NH2	4:D:3777:HOH:O	2.29	0.63
1:C:51:VAL:HG12	1:C:93:ILE:HD13	1.80	0.63
2:G:32:LEU:HD22	2:G:33:PRO:HD2	1.79	0.63
1:A:219:GLN:NE2	1:A:222:ARG:HD3	2.14	0.62
2:H:20:ILE:HD11	4:H:1440:HOH:O	1.98	0.62
1:A:226:THR:HG21	4:A:3511:HOH:O	1.99	0.62
1:A:156:SER:HA	1:A:160:MET:HE3	1.79	0.62
1:C:119:LEU:HB3	1:C:152:ALA:HB2	1.80	0.62
1:A:213:ASP:HB3	2:E:89:ARG:HG3	1.80	0.62
2:H:168:TYR:HB2	2:H:191:MET:HE2	1.82	0.62
1:D:219:GLN:NE2	1:D:222:ARG:HD3	2.15	0.62
1:B:119:LEU:HB3	1:B:152:ALA:HB2	1.82	0.61
1:A:210:SER:HB2	1:A:212:LYS:HZ3	1.65	0.61
1:D:156:SER:HA	1:D:160:MET:HE3	1.82	0.61
1:D:100:LEU:HD13	4:D:4194:HOH:O	2.01	0.61
2:E:32:LEU:HD22	2:E:33:PRO:HD2	1.81	0.61
1:A:226:THR:CG2	4:A:3511:HOH:O	2.46	0.61
1:C:136:ASP:HB3	4:C:2713:HOH:O	1.99	0.61
2:H:32:LEU:HD22	2:H:33:PRO:HD2	1.83	0.61
1:B:68:LYS:NZ	2:F:22:GLY:HA2	2.16	0.61
1:B:116:VAL:HG23	1:B:152:ALA:HB1	1.83	0.61
1:D:195:ALA:HA	4:D:4520:HOH:O	2.01	0.61
2:F:152:ALA:N	4:F:3059:HOH:O	2.34	0.60
2:F:168:TYR:HB2	2:F:191:MET:HE2	1.83	0.60
1:C:104:PHE:HB3	4:C:2676:HOH:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:HB3	2:F:89:ARG:HG3	1.82	0.60
1:C:161:GLN:HE21	1:C:209:GLU:HB3	1.67	0.60
1:B:51:VAL:HG12	1:B:93:ILE:HD13	1.82	0.60
1:B:216:LEU:HD23	2:F:88:GLY:HA2	1.82	0.60
1:C:116:VAL:HG23	1:C:152:ALA:HB1	1.84	0.60
2:H:143:TYR:O	2:H:147:VAL:HG22	2.02	0.60
1:D:211:TYR:O	1:D:212:LYS:HG2	2.01	0.59
1:A:101:LEU:HA	1:A:105:LEU:HB2	1.83	0.59
1:D:75:LYS:HA	1:D:78:MET:HE3	1.85	0.59
2:E:143:TYR:O	2:E:147:VAL:HG22	2.02	0.59
1:C:212:LYS:HA	4:C:2423:HOH:O	2.01	0.59
1:D:119:LEU:HB3	1:D:152:ALA:HB2	1.85	0.59
1:A:73:GLU:N	4:A:2487:HOH:O	2.34	0.59
1:C:101:LEU:HA	1:C:105:LEU:HB2	1.84	0.59
2:F:143:TYR:O	2:F:147:VAL:HG22	2.03	0.59
2:G:143:TYR:O	2:G:147:VAL:HG22	2.02	0.59
1:C:12:LEU:HD21	1:D:79:ALA:HA	1.84	0.58
1:D:101:LEU:HA	1:D:105:LEU:HB2	1.84	0.58
1:A:116:VAL:HG23	1:A:152:ALA:HB1	1.85	0.58
1:D:127:ARG:NH2	2:H:31:TPO:O1P	2.37	0.58
1:A:66:GLU:HG2	1:A:76:GLN:NE2	2.18	0.58
1:D:74:LYS:HB3	4:D:3157:HOH:O	2.03	0.58
1:D:51:VAL:HG12	1:D:93:ILE:HD13	1.84	0.58
1:D:213:ASP:HB3	2:H:89:ARG:HG3	1.85	0.58
1:C:78:MET:HE1	1:D:12:LEU:HD23	1.85	0.58
1:D:116:VAL:HG23	1:D:152:ALA:HB1	1.85	0.57
1:B:101:LEU:HA	1:B:105:LEU:HB2	1.87	0.57
1:D:116:VAL:CG1	1:D:160:MET:HE1	2.34	0.57
2:F:53:ARG:HA	2:F:57:ILE:HD12	1.86	0.57
1:D:35:GLU:HA	4:D:4441:HOH:O	2.04	0.57
1:C:70:GLU:OE2	2:H:170:ARG:HD2	2.05	0.56
1:C:219:GLN:NE2	1:C:222:ARG:HD3	2.20	0.56
2:F:115:ARG:HE	2:G:103:ARG:NH2	2.03	0.56
1:A:133:ALA:HB3	1:A:138:LYS:HD2	1.87	0.56
1:D:74:LYS:HG3	1:D:78:MET:HE2	1.86	0.56
2:E:159:MET:CE	4:E:3297:HOH:O	2.42	0.56
2:H:44:ASP:O	2:H:48:VAL:HG23	2.05	0.56
1:D:138:LYS:O	1:D:142:VAL:HG23	2.06	0.55
1:B:219:GLN:NE2	1:B:222:ARG:HD3	2.22	0.55
1:D:53:GLY:CA	4:D:3872:HOH:O	2.54	0.55
2:E:80:LEU:HD11	2:E:98:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:LYS:HA	1:D:74:LYS:NZ	2.22	0.55
2:G:100:ASP:HA	2:G:117:HIS:CE1	2.42	0.55
2:E:25:GLY:O	2:F:196:ARG:HB3	2.07	0.55
2:F:109:LEU:HD21	2:F:159:MET:HE1	1.89	0.55
2:H:109:LEU:HD21	2:H:159:MET:HE1	1.88	0.54
1:D:219:GLN:HE22	1:D:222:ARG:HD3	1.73	0.54
2:F:157:VAL:HG12	2:F:192:HIS:CD2	2.42	0.54
1:A:138:LYS:O	1:A:142:VAL:HG23	2.08	0.54
1:C:83:ARG:O	1:C:87:GLU:HG3	2.08	0.54
1:D:113:GLU:HG2	1:D:166:ILE:HD12	1.89	0.54
1:A:15:GLN:HG3	4:A:3061:HOH:O	2.07	0.54
1:D:207:SER:C	1:D:209:GLU:H	2.16	0.54
2:F:80:LEU:HD11	2:F:98:LEU:HG	1.89	0.54
1:A:58:SER:O	1:A:62:VAL:HG12	2.09	0.53
1:A:74:LYS:O	1:A:74:LYS:HG3	2.07	0.53
2:G:80:LEU:HD11	2:G:98:LEU:HG	1.89	0.53
2:E:100:ASP:HA	2:E:117:HIS:CE1	2.43	0.53
1:A:75:LYS:HD3	1:A:78:MET:CG	2.39	0.53
1:A:75:LYS:CD	1:A:78:MET:HG3	2.39	0.53
1:C:58:SER:O	1:C:62:VAL:HG12	2.09	0.53
1:D:39:GLU:HB2	4:D:4270:HOH:O	2.08	0.53
2:H:100:ASP:HA	2:H:117:HIS:CE1	2.43	0.53
1:A:74:LYS:O	1:A:76:GLN:N	2.43	0.52
2:G:180:ALA:CB	4:G:3032:HOH:O	2.57	0.52
2:H:80:LEU:HD11	2:H:98:LEU:HG	1.92	0.52
1:A:219:GLN:HE22	1:A:222:ARG:HD3	1.74	0.52
1:A:100:LEU:CD1	4:A:3264:HOH:O	2.57	0.52
2:F:100:ASP:HA	2:F:117:HIS:CE1	2.45	0.52
2:F:152:ALA:CB	4:F:3059:HOH:O	2.57	0.52
2:E:109:LEU:HD21	2:E:159:MET:HE1	1.92	0.52
1:A:73:GLU:C	4:A:2487:HOH:O	2.53	0.51
1:D:83:ARG:O	1:D:87:GLU:HG3	2.10	0.51
1:C:113:GLU:HB2	4:C:2183:HOH:O	2.09	0.51
1:A:161:GLN:HE21	1:A:209:GLU:HB3	1.76	0.51
1:B:116:VAL:CG1	1:B:160:MET:HE1	2.38	0.51
1:C:94:CYS:HB2	1:C:129:LEU:HD13	1.93	0.51
1:C:138:LYS:O	1:C:142:VAL:HG23	2.11	0.51
1:B:116:VAL:HG11	1:B:160:MET:CE	2.40	0.51
1:D:58:SER:O	1:D:62:VAL:HG12	2.11	0.51
2:H:77:CYS:HB2	2:H:80:LEU:HD12	1.93	0.50
1:A:70:GLU:CD	2:F:170:ARG:HD2	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLU:HG2	1:A:166:ILE:HD12	1.93	0.50
1:D:212:LYS:HA	4:D:4321:HOH:O	2.09	0.50
2:G:77:CYS:HB2	2:G:80:LEU:HD12	1.94	0.50
2:G:157:VAL:HG12	2:G:192:HIS:CD2	2.46	0.50
2:F:75:THR:HB	2:G:185:SER:HB3	1.94	0.50
2:H:31:TPO:O1P	2:H:31:TPO:HG21	2.12	0.50
1:C:80:ARG:O	1:C:84:GLU:HG3	2.12	0.50
1:B:59:TRP:CE2	1:B:132:VAL:HG12	2.47	0.50
1:C:74:LYS:HD3	1:C:74:LYS:H	1.71	0.49
1:A:14:GLU:HB3	4:A:3061:HOH:O	2.11	0.49
1:A:116:VAL:CG1	1:A:160:MET:HE1	2.38	0.49
1:B:58:SER:O	1:B:62:VAL:HG12	2.12	0.49
2:G:25:GLY:O	2:H:196:ARG:HB3	2.12	0.49
1:A:83:ARG:O	1:A:87:GLU:HG3	2.12	0.49
1:B:127:ARG:NH2	2:F:31:TPO:O1P	2.45	0.49
2:G:24:PRO:HB3	2:H:144:LEU:C	2.38	0.49
2:H:157:VAL:HG12	2:H:192:HIS:CD2	2.48	0.49
1:A:70:GLU:OE2	2:F:170:ARG:HD2	2.12	0.49
1:C:213:ASP:HB3	2:G:89:ARG:HG3	1.95	0.49
2:G:115:ARG:HA	4:G:3337:HOH:O	2.11	0.49
1:A:115:LYS:O	1:A:119:LEU:HB2	2.13	0.49
2:G:109:LEU:HD21	2:G:159:MET:HE1	1.94	0.48
1:C:113:GLU:HG2	1:C:166:ILE:HD12	1.95	0.48
1:D:176:VAL:HG13	2:H:29:ARG:HD2	1.96	0.48
2:F:167:PHE:O	2:F:170:ARG:HG3	2.14	0.48
1:A:77:GLN:O	1:A:81:GLU:HG3	2.14	0.48
1:C:210:SER:HB2	1:C:212:LYS:NZ	2.27	0.48
1:C:219:GLN:HE22	1:C:222:ARG:HD3	1.78	0.48
1:C:161:GLN:NE2	1:C:209:GLU:O	2.47	0.48
1:A:30:THR:HG23	4:A:3467:HOH:O	2.13	0.48
1:B:168:LEU:CD1	4:B:1726:HOH:O	2.61	0.48
1:C:59:TRP:CE2	1:C:132:VAL:HG12	2.48	0.48
1:C:116:VAL:CG1	1:C:160:MET:HE1	2.43	0.48
2:G:155:ARG:HG2	2:G:156:ALA:N	2.28	0.48
1:C:8:GLN:HG2	1:D:78:MET:HE1	1.95	0.48
1:D:74:LYS:HA	1:D:74:LYS:HZ2	1.79	0.48
1:D:80:ARG:O	1:D:84:GLU:HG3	2.14	0.48
2:E:157:VAL:HG12	2:E:192:HIS:CD2	2.48	0.48
1:D:59:TRP:CE2	1:D:132:VAL:HG12	2.49	0.48
1:A:116:VAL:HG11	1:A:160:MET:CE	2.41	0.47
1:D:115:LYS:O	1:D:119:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:20:ILE:CG2	2:E:23:SER:HB2	2.44	0.47
2:E:138:VAL:O	2:E:142:ARG:HB2	2.15	0.47
1:A:35:GLU:OE1	4:A:3725:HOH:O	2.19	0.47
1:B:108:ASN:HB2	4:B:1727:HOH:O	2.14	0.47
2:H:167:PHE:O	2:H:170:ARG:HG3	2.14	0.47
1:A:75:LYS:NZ	1:B:5:GLU:HG2	2.30	0.47
2:F:31:TPO:O1P	2:F:31:TPO:HG21	2.15	0.47
1:A:94:CYS:HB2	1:A:129:LEU:HD13	1.95	0.47
1:B:150:GLN:HB3	4:B:1438:HOH:O	2.15	0.47
1:D:98:LEU:HD12	1:D:98:LEU:HA	1.83	0.47
2:F:105:THR:O	2:F:108:SER:OG	2.33	0.47
2:F:157:VAL:HG12	2:F:192:HIS:HD2	1.80	0.47
1:B:94:CYS:HB2	1:B:129:LEU:HD13	1.97	0.46
1:D:94:CYS:HB2	1:D:129:LEU:HD13	1.98	0.46
2:F:77:CYS:HB2	2:F:80:LEU:HD12	1.96	0.46
1:A:127:ARG:NH2	2:E:31:TPO:O1P	2.49	0.46
4:A:3431:HOH:O	2:E:32:LEU:HB3	2.15	0.46
1:B:219:GLN:HE22	1:B:222:ARG:HD3	1.79	0.46
2:F:20:ILE:CG2	2:F:23:SER:HB2	2.44	0.46
1:B:55:ARG:HB3	1:B:90:LEU:HD13	1.98	0.46
1:B:83:ARG:O	1:B:87:GLU:HG3	2.16	0.46
1:B:186:GLU:H	1:B:186:GLU:CD	2.23	0.46
2:E:155:ARG:HG2	2:E:156:ALA:N	2.30	0.46
2:G:20:ILE:CG2	2:G:23:SER:HB2	2.44	0.46
2:G:133:GLN:HB3	2:G:135:LYS:HE2	1.98	0.46
2:H:32:LEU:HD11	2:H:87:GLU:HB3	1.96	0.46
2:E:132:GLN:HE22	3:E:401:COT:HC8	1.81	0.46
2:F:152:ALA:HB2	4:F:3059:HOH:O	2.15	0.46
1:D:106:ILE:CG1	1:D:107:PRO:HD3	2.46	0.46
2:E:77:CYS:HB2	2:E:80:LEU:HD12	1.98	0.46
2:H:105:THR:O	2:H:108:SER:OG	2.33	0.46
1:A:186:GLU:CD	1:A:186:GLU:H	2.24	0.46
1:C:162:PRO:HG2	4:C:2035:HOH:O	2.15	0.46
1:D:201:ALA:O	1:D:204:ASP:HB2	2.16	0.46
2:F:155:ARG:HG2	2:F:156:ALA:N	2.31	0.46
1:C:94:CYS:CB	1:C:129:LEU:HD13	2.46	0.46
1:C:186:GLU:CD	1:C:186:GLU:H	2.23	0.46
2:F:44:ASP:O	2:F:48:VAL:HG23	2.16	0.46
1:A:49:LYS:HE3	1:A:128:TYR:OH	2.16	0.45
1:B:94:CYS:CB	1:B:129:LEU:HD13	2.45	0.45
1:A:75:LYS:HE3	1:B:8:GLN:CB	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:LYS:HD3	1:A:78:MET:HG3	1.98	0.45
2:F:115:ARG:NE	2:G:103:ARG:NH2	2.64	0.45
1:A:12:LEU:HD21	1:B:79:ALA:HA	1.98	0.45
1:C:115:LYS:O	1:C:119:LEU:HB2	2.16	0.45
1:A:79:ALA:HA	1:B:12:LEU:HD21	1.97	0.45
1:B:55:ARG:CB	1:B:90:LEU:HD13	2.46	0.45
1:D:116:VAL:HG11	1:D:160:MET:CE	2.39	0.45
2:H:138:VAL:O	2:H:142:ARG:HB2	2.16	0.45
2:H:155:ARG:HG2	2:H:156:ALA:N	2.32	0.45
1:B:80:ARG:O	1:B:84:GLU:HG3	2.17	0.45
2:F:138:VAL:O	2:F:142:ARG:HB2	2.17	0.45
2:E:62:ASN:ND2	2:E:184:GLY:HA3	2.32	0.44
2:G:34:ALA:HA	2:G:87:GLU:HG2	1.98	0.44
2:G:138:VAL:O	2:G:142:ARG:HB2	2.17	0.44
2:G:161:GLU:H	2:G:161:GLU:HG2	1.54	0.44
1:B:78:MET:HE2	1:B:78:MET:HA	1.99	0.44
2:E:161:GLU:H	2:E:161:GLU:HG2	1.56	0.44
2:G:159:MET:HE2	4:G:2903:HOH:O	2.15	0.44
1:B:49:LYS:HE3	1:B:128:TYR:OH	2.17	0.44
2:H:150:GLN:HA	2:H:151:PRO:HD3	1.59	0.44
2:H:165:VAL:HB	2:H:166:PRO:HD3	1.99	0.44
2:H:34:ALA:HA	2:H:87:GLU:HG2	2.00	0.44
1:A:59:TRP:CE2	1:A:132:VAL:HG12	2.53	0.44
1:D:149:TYR:HB3	1:D:174:PHE:CE1	2.53	0.44
1:D:186:GLU:H	1:D:186:GLU:CD	2.26	0.44
2:F:23:SER:HB3	2:F:26:ARG:HD3	2.00	0.44
2:G:132:GLN:HE22	3:G:402:COT:HC8	1.83	0.44
2:H:20:ILE:CG2	2:H:23:SER:HB2	2.47	0.44
1:A:212:LYS:HE2	4:A:3846:HOH:O	2.17	0.44
1:D:216:LEU:HD23	2:H:88:GLY:HA2	2.00	0.44
2:F:165:VAL:HB	2:F:166:PRO:HD3	2.00	0.44
1:A:157:LYS:HE2	4:A:4240:HOH:O	2.17	0.44
4:A:3846:HOH:O	2:E:50:GLU:HG3	2.16	0.44
1:C:49:LYS:HE3	1:C:128:TYR:OH	2.17	0.44
2:E:100:ASP:C	2:E:117:HIS:HE1	2.25	0.44
2:G:31:TPO:O1P	2:G:31:TPO:HG21	2.17	0.44
2:G:53:ARG:HA	2:G:57:ILE:HD12	1.99	0.44
1:B:168:LEU:HD11	4:B:1726:HOH:O	2.18	0.44
1:B:113:GLU:HG2	1:B:166:ILE:HD12	2.00	0.43
2:G:29:ARG:H	2:G:29:ARG:HG3	1.60	0.43
2:G:100:ASP:C	2:G:117:HIS:HE1	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:180:ALA:HB3	4:G:3032:HOH:O	2.18	0.43
2:E:167:PHE:O	2:E:170:ARG:HG3	2.18	0.43
2:G:150:GLN:HA	2:G:151:PRO:HD3	1.60	0.43
2:G:165:VAL:HB	2:G:166:PRO:HD3	1.99	0.43
1:B:106:ILE:CG1	1:B:107:PRO:HD3	2.49	0.43
1:C:119:LEU:HD12	1:C:119:LEU:HA	1.86	0.43
2:E:34:ALA:HA	2:E:87:GLU:HG2	1.99	0.43
1:A:68:LYS:O	1:A:69:THR:C	2.60	0.43
1:A:106:ILE:CG1	1:A:107:PRO:HD3	2.48	0.43
1:A:199:ALA:HB3	1:A:218:MET:HE3	2.01	0.43
1:A:80:ARG:O	1:A:84:GLU:HG3	2.17	0.43
1:B:115:LYS:O	1:B:119:LEU:HB2	2.19	0.43
2:E:145:HIS:CE1	2:F:24:PRO:HA	2.54	0.43
1:C:42:ASN:ND2	2:G:86:VAL:HG13	2.34	0.43
2:E:150:GLN:HA	2:E:151:PRO:HD3	1.60	0.43
2:E:183:VAL:O	2:E:186:LEU:HB2	2.19	0.43
2:G:167:PHE:O	2:G:170:ARG:HG3	2.19	0.43
1:D:55:ARG:CB	1:D:90:LEU:HD13	2.49	0.42
2:F:122:HIS:O	3:F:400:COT:H2T1	2.19	0.42
1:D:94:CYS:CB	1:D:129:LEU:HD13	2.49	0.42
2:E:31:TPO:O1P	2:E:31:TPO:HG21	2.18	0.42
2:F:100:ASP:C	2:F:117:HIS:HE1	2.28	0.42
2:H:100:ASP:C	2:H:117:HIS:HE1	2.27	0.42
2:H:161:GLU:H	2:H:161:GLU:HG2	1.55	0.42
1:C:127:ARG:NH2	2:G:31:TPO:O1P	2.53	0.42
2:E:46:ALA:O	2:E:50:GLU:HG2	2.19	0.42
2:G:158:LEU:HD12	2:G:158:LEU:C	2.44	0.42
2:E:158:LEU:C	2:E:158:LEU:HD12	2.45	0.42
1:C:116:VAL:HG11	1:C:160:MET:CE	2.45	0.42
1:A:94:CYS:CB	1:A:129:LEU:HD13	2.49	0.42
1:A:216:LEU:HD23	2:E:88:GLY:HA2	2.02	0.42
1:D:225:LEU:HD12	1:D:225:LEU:HA	1.96	0.42
1:D:211:TYR:C	1:D:212:LYS:HG2	2.45	0.42
2:G:23:SER:HB3	2:G:26:ARG:HD3	2.00	0.41
1:A:72:ALA:H	1:A:74:LYS:HZ2	1.68	0.41
1:A:210:SER:HB2	1:A:212:LYS:HZ2	1.83	0.41
1:B:20:ASP:CG	4:B:2532:HOH:O	2.63	0.41
1:D:101:LEU:O	1:D:106:ILE:HG12	2.20	0.41
2:E:34:ALA:O	2:E:35:ASN:HB2	2.20	0.41
1:A:11:LYS:O	4:A:3061:HOH:O	2.22	0.41
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLU:HA	4:B:1794:HOH:O	2.20	0.41
1:C:121:MET:O	1:C:125:TYR:HD1	2.03	0.41
1:C:130:ALA:HA	1:C:133:ALA:HB2	2.03	0.41
2:H:26:ARG:N	2:H:26:ARG:CD	2.84	0.41
1:D:144:GLN:CG	4:D:4412:HOH:O	2.21	0.41
2:F:115:ARG:HE	2:G:103:ARG:HH21	1.69	0.41
2:H:20:ILE:HD11	2:H:28:ARG:HA	2.01	0.41
1:A:46:VAL:HG21	2:E:35:ASN:CG	2.45	0.41
1:B:149:TYR:HB3	1:B:174:PHE:CE1	2.55	0.41
2:E:20:ILE:HD11	2:E:28:ARG:HA	2.02	0.41
2:E:94:ILE:HG12	2:E:124:LEU:HD13	2.01	0.41
2:G:115:ARG:HD3	4:G:3362:HOH:O	2.16	0.41
1:A:71:GLY:HA3	1:A:74:LYS:HZ2	1.86	0.41
1:C:216:LEU:HD23	2:G:88:GLY:HA2	2.01	0.41
2:F:26:ARG:N	2:F:26:ARG:CD	2.84	0.41
2:H:53:ARG:HA	2:H:57:ILE:HD12	2.03	0.41
2:G:78:PRO:HB2	4:G:2927:HOH:O	2.21	0.41
1:C:199:ALA:HB3	1:C:218:MET:HE3	2.02	0.41
1:C:61:VAL:HG11	1:D:16:ALA:HA	2.02	0.41
1:C:225:LEU:HD12	1:C:225:LEU:HA	1.95	0.41
1:D:113:GLU:CG	1:D:166:ILE:HD12	2.51	0.41
2:E:165:VAL:HB	2:E:166:PRO:HD3	2.02	0.41
2:F:150:GLN:HA	2:F:151:PRO:HD3	1.63	0.41
2:G:132:GLN:NE2	4:G:2717:HOH:O	2.49	0.41
2:H:23:SER:HB3	2:H:26:ARG:HD3	2.02	0.41
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.88	0.41
1:D:180:GLU:OE2	2:H:29:ARG:HD3	2.20	0.41
2:F:29:ARG:H	2:F:29:ARG:HG3	1.63	0.41
2:F:32:LEU:HD11	2:F:87:GLU:HB3	2.03	0.41
2:G:173:PHE:HB3	2:G:191:MET:HB3	2.03	0.40
1:B:199:ALA:HB3	1:B:218:MET:HE3	2.02	0.40
1:C:106:ILE:CG1	1:C:107:PRO:HD3	2.51	0.40
2:H:84:TRP:HZ3	2:H:138:VAL:HB	1.85	0.40
1:A:49:LYS:HG2	2:E:34:ALA:HB2	2.02	0.40
1:C:106:ILE:HG12	1:C:107:PRO:HD3	2.03	0.40
2:H:159:MET:HG2	4:H:1299:HOH:O	2.20	0.40
1:C:98:LEU:HD12	1:C:98:LEU:HA	1.84	0.40
2:F:30:HIS:HA	4:F:2192:HOH:O	2.22	0.40
2:H:29:ARG:H	2:H:29:ARG:HG3	1.59	0.40
2:F:52:GLU:OE2	2:F:64:PRO:HD2	2.21	0.40
2:G:80:LEU:HD13	2:G:97:SER:HA	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:177:GLY:N	4:C:2713:HOH:O[1_554]	2.05	0.15
1:B:31:GLU:O	4:D:4373:HOH:O[1_464]	2.09	0.11

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	225/245 (92%)	216 (96%)	8 (4%)	1 (0%)	30	54
1	B	225/245 (92%)	215 (96%)	8 (4%)	2 (1%)	14	35
1	C	225/245 (92%)	218 (97%)	6 (3%)	1 (0%)	30	54
1	D	225/245 (92%)	216 (96%)	9 (4%)	0	100	100
2	E	176/200 (88%)	167 (95%)	7 (4%)	2 (1%)	11	29
2	F	176/200 (88%)	169 (96%)	5 (3%)	2 (1%)	11	29
2	G	176/200 (88%)	169 (96%)	5 (3%)	2 (1%)	11	29
2	H	176/200 (88%)	168 (96%)	6 (3%)	2 (1%)	11	29
All	All	1604/1780 (90%)	1538 (96%)	54 (3%)	12 (1%)	18	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	ALA
1	C	134	ALA
1	A	75	LYS
2	E	151	PRO
2	F	151	PRO
2	G	151	PRO
2	H	151	PRO
1	B	211	TYR

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Mol	Chain	Res	Type
2	H	35	ASN
2	E	35	ASN
2	F	35	ASN
2	G	35	ASN

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	197/209 (94%)	172 (87%)	25 (13%)	4	11
1	B	197/209 (94%)	176 (89%)	21 (11%)	6	16
1	C	197/209 (94%)	173 (88%)	24 (12%)	5	12
1	D	197/209 (94%)	174 (88%)	23 (12%)	5	13
2	E	148/166 (89%)	140 (95%)	8 (5%)	20	45
2	F	148/166 (89%)	141 (95%)	7 (5%)	23	51
2	G	148/166 (89%)	141 (95%)	7 (5%)	23	51
2	H	148/166 (89%)	140 (95%)	8 (5%)	20	45
All	All	1380/1500 (92%)	1257 (91%)	123 (9%)	9	23

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	8	GLN
1	A	43	LEU
1	A	67	GLN
1	A	70	GLU
1	A	77	GLN
1	A	91	ARG
1	A	96	ASP
1	A	97	VAL
1	A	98	LEU
1	A	100	LEU

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Mol	Chain	Res	Type
1	A	101	LEU
1	A	102	GLU
1	A	105	LEU
1	A	114	SER
1	A	119	LEU
1	A	154	GLU
1	A	156	SER
1	A	168	LEU
1	A	182	LEU
1	A	187	LYS
1	A	191	LEU
1	A	212	LYS
1	A	220	LEU
1	A	225	LEU
1	B	6	LEU
1	B	36	LEU
1	B	43	LEU
1	B	91	ARG
1	B	96	ASP
1	B	97	VAL
1	B	98	LEU
1	B	100	LEU
1	B	101	LEU
1	B	102	GLU
1	B	105	LEU
1	B	114	SER
1	B	119	LEU
1	B	136	ASP
1	B	154	GLU
1	B	156	SER
1	B	168	LEU
1	B	182	LEU
1	B	187	LYS
1	B	191	LEU
1	B	225	LEU
1	C	6	LEU
1	C	36	LEU
1	C	43	LEU
1	C	67	GLN
1	C	74	LYS
1	C	78	MET
1	C	91	ARG

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Mol	Chain	Res	Type
1	C	96	ASP
1	C	97	VAL
1	C	98	LEU
1	C	100	LEU
1	C	101	LEU
1	C	105	LEU
1	C	114	SER
1	C	119	LEU
1	C	154	GLU
1	C	156	SER
1	C	168	LEU
1	C	182	LEU
1	C	187	LYS
1	C	191	LEU
1	C	210	SER
1	C	212	LYS
1	C	225	LEU
1	D	6	LEU
1	D	36	LEU
1	D	43	LEU
1	D	67	GLN
1	D	69	THR
1	D	74	LYS
1	D	91	ARG
1	D	96	ASP
1	D	97	VAL
1	D	98	LEU
1	D	100	LEU
1	D	101	LEU
1	D	102	GLU
1	D	105	LEU
1	D	114	SER
1	D	119	LEU
1	D	154	GLU
1	D	156	SER
1	D	168	LEU
1	D	182	LEU
1	D	191	LEU
1	D	212	LYS
1	D	225	LEU
2	E	29	ARG
2	E	32	LEU

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Mol	Chain	Res	Type
2	E	60	SER
2	E	62	ASN
2	E	67	LEU
2	E	76	LEU
2	E	139	LEU
2	E	161	GLU
2	F	29	ARG
2	F	32	LEU
2	F	60	SER
2	F	67	LEU
2	F	76	LEU
2	F	139	LEU
2	F	161	GLU
2	G	29	ARG
2	G	32	LEU
2	G	60	SER
2	G	67	LEU
2	G	76	LEU
2	G	139	LEU
2	G	161	GLU
2	H	27	GLN
2	H	29	ARG
2	H	32	LEU
2	H	60	SER
2	H	67	LEU
2	H	76	LEU
2	H	139	LEU
2	H	161	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	108	ASN
1	A	146	GLN
1	A	161	GLN
1	A	219	GLN
1	B	8	GLN
1	B	42	ASN
1	B	76	GLN
1	B	77	GLN
1	B	108	ASN

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Mol	Chain	Res	Type
1	B	219	GLN
1	C	42	ASN
1	C	76	GLN
1	C	77	GLN
1	C	108	ASN
1	C	146	GLN
1	C	161	GLN
1	C	219	GLN
1	D	4	ASN
1	D	42	ASN
1	D	108	ASN
1	D	146	GLN
1	D	219	GLN
2	E	35	ASN
2	E	62	ASN
2	E	117	HIS
2	E	132	GLN
2	F	35	ASN
2	F	62	ASN
2	F	117	HIS
2	F	132	GLN
2	G	35	ASN
2	G	62	ASN
2	G	117	HIS
2	G	132	GLN
2	H	35	ASN
2	H	62	ASN
2	H	117	HIS
2	H	132	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	TPO	F	31	2	8,10,11	1.19	0	10,14,16	1.22	0
2	TPO	G	31	2	8,10,11	1.35	2 (25%)	10,14,16	1.31	1 (10%)
2	TPO	E	31	2	8,10,11	1.46	2 (25%)	10,14,16	1.22	0
2	TPO	H	31	2	8,10,11	1.52	2 (25%)	10,14,16	1.25	1 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPO	F	31	2	-	1/9/11/13	-
2	TPO	G	31	2	-	1/9/11/13	-
2	TPO	E	31	2	-	1/9/11/13	-
2	TPO	H	31	2	-	1/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	31	TPO	P-O2P	-2.48	1.45	1.54
2	E	31	TPO	P-O3P	-2.39	1.45	1.54
2	G	31	TPO	P-O2P	-2.39	1.45	1.54
2	H	31	TPO	P-OG1	-2.33	1.55	1.59
2	E	31	TPO	P-O2P	-2.24	1.46	1.54
2	G	31	TPO	P-O3P	-2.11	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	31	TPO	P-OG1-CB	-2.21	117.31	123.33
2	H	31	TPO	P-OG1-CB	-2.11	117.58	123.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	31	TPO	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
2	F	31	TPO	O-C-CA-CB
2	G	31	TPO	O-C-CA-CB
2	H	31	TPO	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	31	TPO	2	0
2	G	31	TPO	2	0
2	E	31	TPO	2	0
2	H	31	TPO	2	0

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	COT	H	403	-	65,67,67	0.68	0	92,98,98	0.91	3 (3%)
3	COT	E	401	-	65,67,67	0.72	0	92,98,98	0.91	4 (4%)
3	COT	F	400	-	65,67,67	0.77	1 (1%)	92,98,98	0.90	3 (3%)
3	COT	G	402	-	65,67,67	0.74	2 (3%)	92,98,98	0.89	1 (1%)

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	COT	H	403	-	-	10/58/74/74	0/5/5/5
3	COT	E	401	-	-	10/58/74/74	0/5/5/5
3	COT	F	400	-	-	9/58/74/74	0/5/5/5
3	COT	G	402	-	-	9/58/74/74	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	400	COT	C11-C12	2.23	1.44	1.41
3	G	402	COT	C11-C12	2.22	1.44	1.41
3	G	402	COT	C17-C16	2.07	1.42	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	403	COT	N3A-C2A-N1A	-3.46	123.34	128.58
3	F	400	COT	N3A-C2A-N1A	-3.41	123.41	128.58
3	E	401	COT	N3A-C2A-N1A	-3.34	123.52	128.58
3	G	402	COT	N3A-C2A-N1A	-3.21	123.72	128.58
3	H	403	COT	N9A-C8A-N7A	-2.30	110.67	113.94
3	E	401	COT	N9A-C8A-N7A	-2.24	110.76	113.94
3	E	401	COT	C4A-N9A-C8A	2.19	108.04	105.74
3	F	400	COT	N9A-C8A-N7A	-2.10	110.96	113.94
3	F	400	COT	C4A-N9A-C8A	2.09	107.94	105.74
3	E	401	COT	C1T-C2T-N3T	-2.04	107.67	112.00
3	H	403	COT	C4A-N9A-C8A	2.02	107.86	105.74

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	402	COT	C3B-C4B-C5B-O5B
3	E	401	COT	C3B-C4B-C5B-O5B
3	F	400	COT	C3B-C4B-C5B-O5B
3	H	403	COT	C3B-C4B-C5B-O5B
3	E	401	COT	CGT-C1T-C2T-N3T
3	F	400	COT	CGT-C1T-C2T-N3T
3	G	402	COT	CGT-C1T-C2T-N3T
3	H	403	COT	CGT-C1T-C2T-N3T
3	G	402	COT	N8P-C9P-CBP-OCF
3	F	400	COT	C6P-C7P-N8P-C9P

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Mol	Chain	Res	Type	Atoms
3	G	402	COT	O4B-C4B-C5B-O5B
3	G	402	COT	C6P-C7P-N8P-C9P
3	F	400	COT	O4B-C4B-C5B-O5B
3	E	401	COT	C3B-O3B-PC-O17
3	F	400	COT	C3B-O3B-PC-O17
3	G	402	COT	C3B-O3B-PC-O17
3	H	403	COT	C3B-O3B-PC-O17
3	E	401	COT	O4B-C4B-C5B-O5B
3	H	403	COT	O4B-C4B-C5B-O5B
3	E	401	COT	C6P-C7P-N8P-C9P
3	H	403	COT	C6P-C7P-N8P-C9P
3	E	401	COT	C3B-O3B-PC-O19
3	G	402	COT	C3B-O3B-PC-O19
3	H	403	COT	C3B-O3B-PC-O19
3	G	402	COT	PA-O14-PB-O12
3	E	401	COT	PA-O14-PB-O12
3	E	401	COT	PA-O14-PB-O13
3	F	400	COT	PA-O14-PB-O12
3	F	400	COT	PA-O14-PB-O13
3	G	402	COT	PA-O14-PB-O13
3	H	403	COT	PA-O14-PB-O12
3	H	403	COT	PA-O14-PB-O13
3	E	401	COT	C3B-O3B-PC-O18
3	H	403	COT	C3B-O3B-PC-O18
3	F	400	COT	C3B-O3B-PC-O19
3	E	401	COT	N8P-C9P-CBP-OCP
3	F	400	COT	N8P-C9P-CBP-OCP
3	H	403	COT	N8P-C9P-CBP-OCP

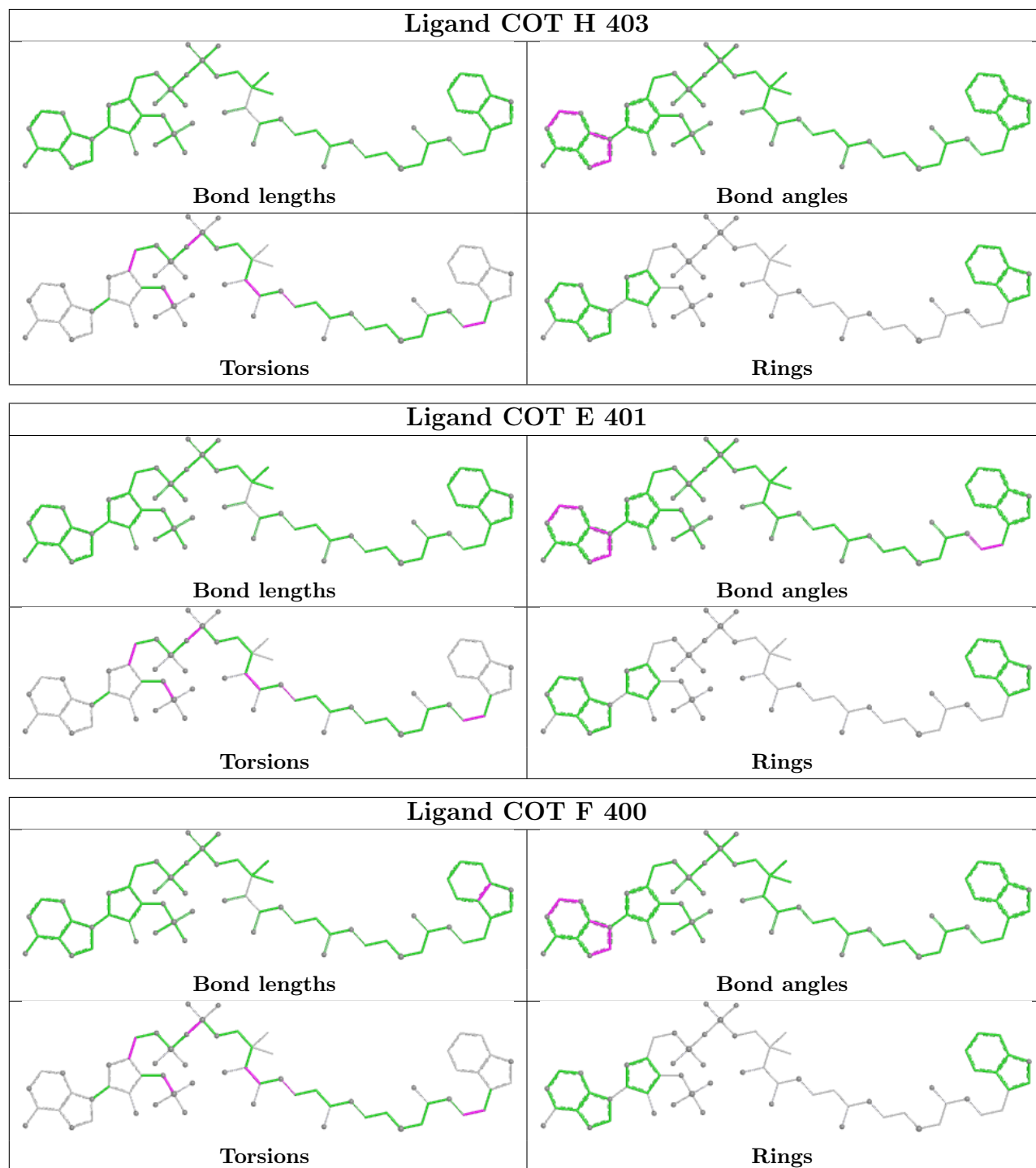
There are no ring outliers.

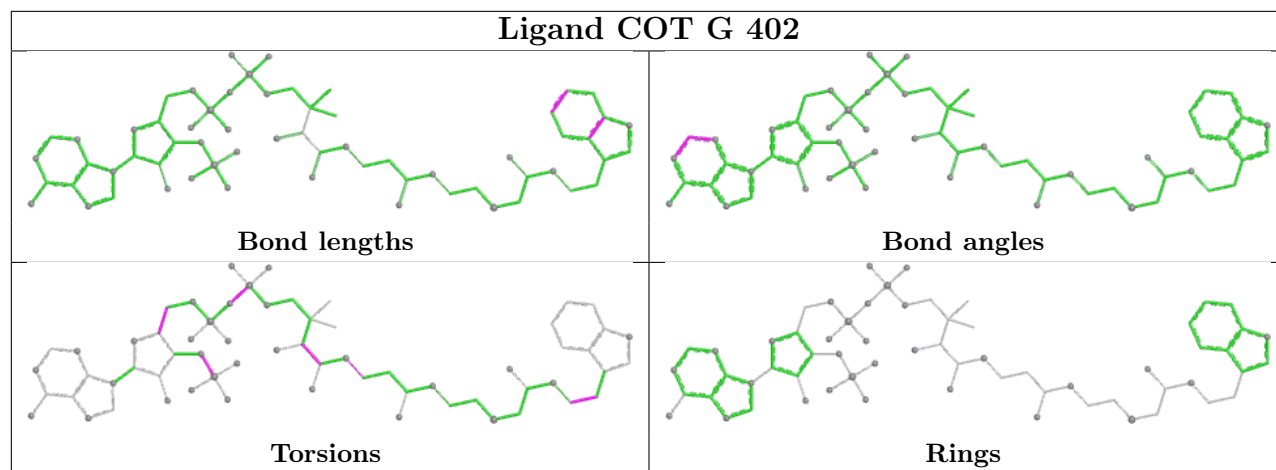
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	401	COT	1	0
3	F	400	COT	1	0
3	G	402	COT	1	0

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

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





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.