



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:14 PM UTC

PDB ID : 1EJI / pdb_00001eji
Title : RECOMBINANT SERINE HYDROXYMETHYLTRANSFERASE
(MOUSE)
Authors : Szebenyi, D.M.E.; Liu, X.; Kriksunov, I.A.; Stover, P.J.; Thiel, D.J.
Deposited on : 2000-03-02
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

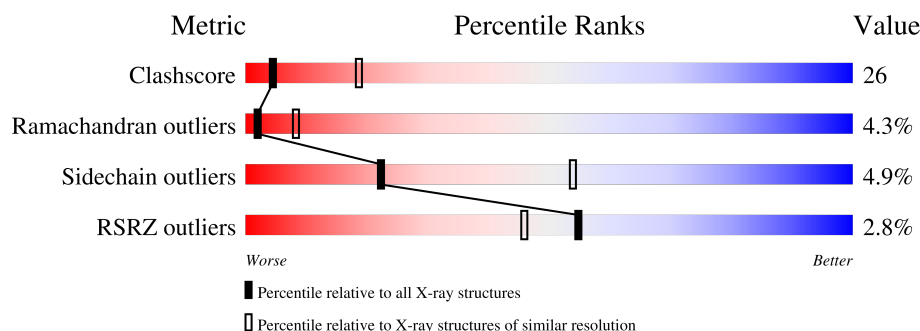
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	478	4% 55% 40% • •
1	B	478	% 57% 37% 5% •
1	C	478	3% 53% 39% 7% •
1	D	478	3% 52% 41% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLG	A	500	-	X	-	-
2	PLG	B	501	-	X	-	-
2	PLG	C	502	-	X	-	-
2	PLG	D	503	-	X	-	-

2 Entry composition [i](#)

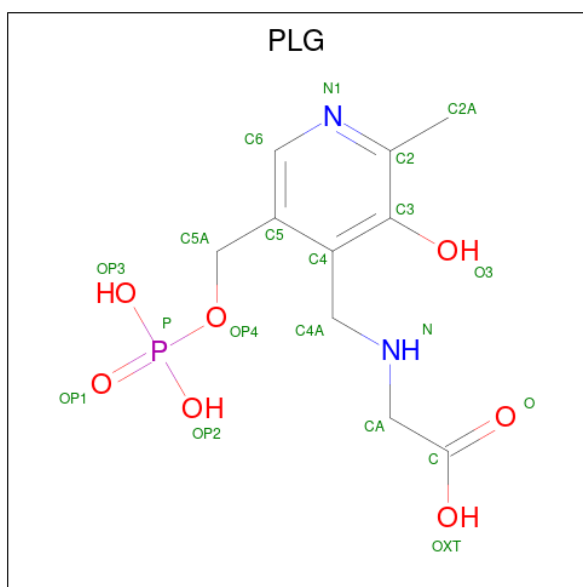
There are 4 unique types of molecules in this entry. The entry contains 14984 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	Se	0	0	0
			3695	2329	641	704	10	11			
1	B	478	Total	C	N	O	S	Se	0	0	0
			3695	2329	641	704	10	11			
1	C	478	Total	C	N	O	S	Se	0	0	0
			3695	2329	641	704	10	11			
1	D	478	Total	C	N	O	S	Se	0	0	0
			3695	2329	641	704	10	11			

- Molecule 2 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL-METHANE] (CCD ID: PLG) (formula: C₁₀H₁₅N₂O₇P).



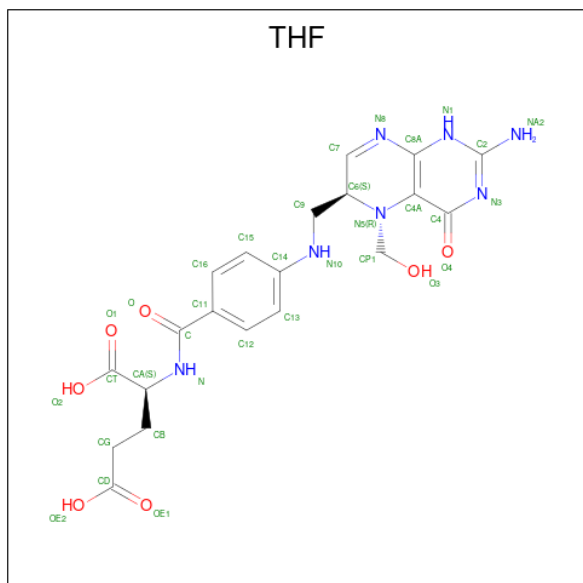
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	B	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			20	10	2	7	1		
2	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 3 is 5-HYDROXYMETHYLENE-6-HYDROFOLIC ACID (CCD ID: THF) (formula: C₂₀H₂₃N₇O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	20	7	7		
3	B	1	Total	C	N	O	0	0
			34	20	7	7		
3	D	1	Total	C	N	O	0	0
			34	20	7	7		

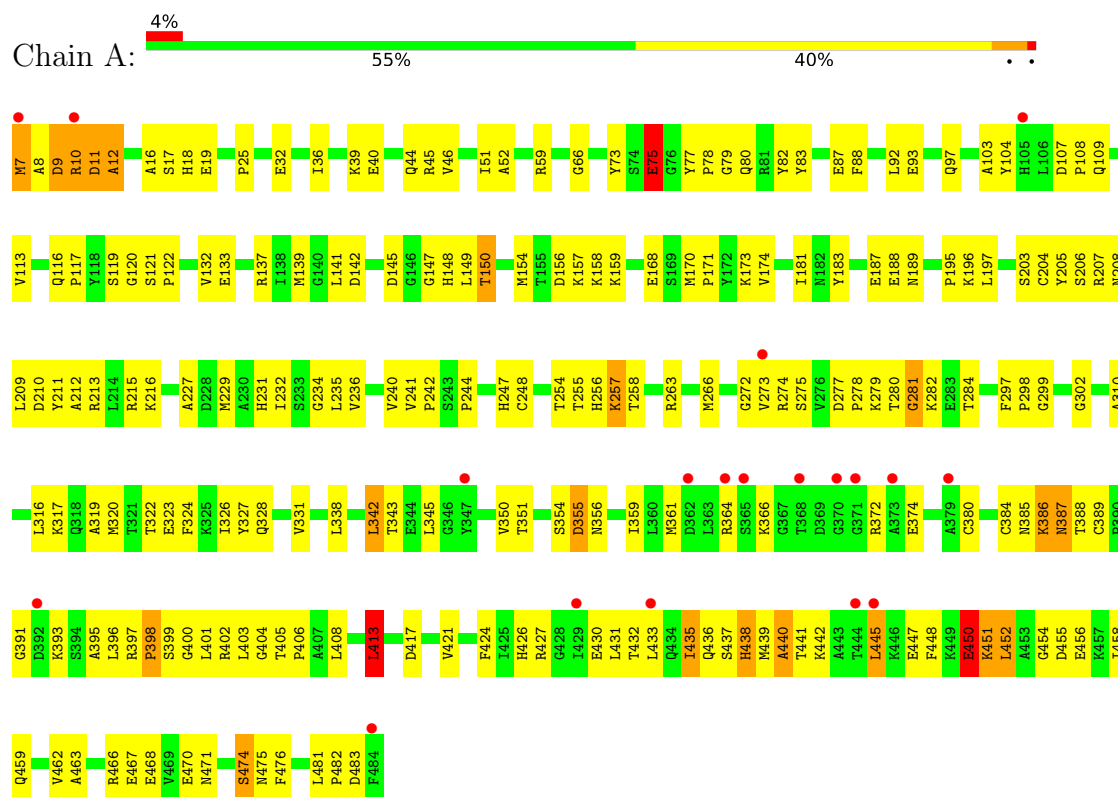
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	4	Total	O	0	0
			4	4		
4	C	9	Total	O	0	0
			9	9		
4	D	4	Total	O	0	0
			4	4		

3 Residue-property plots

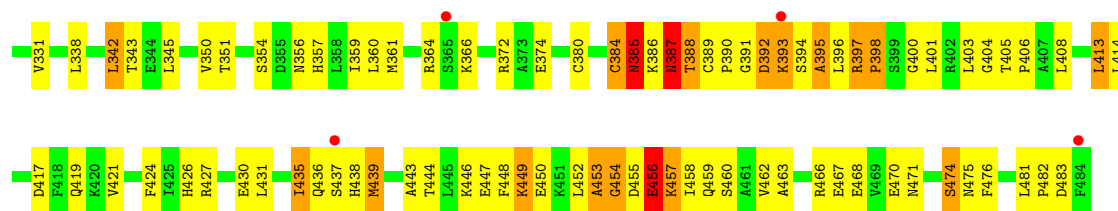
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

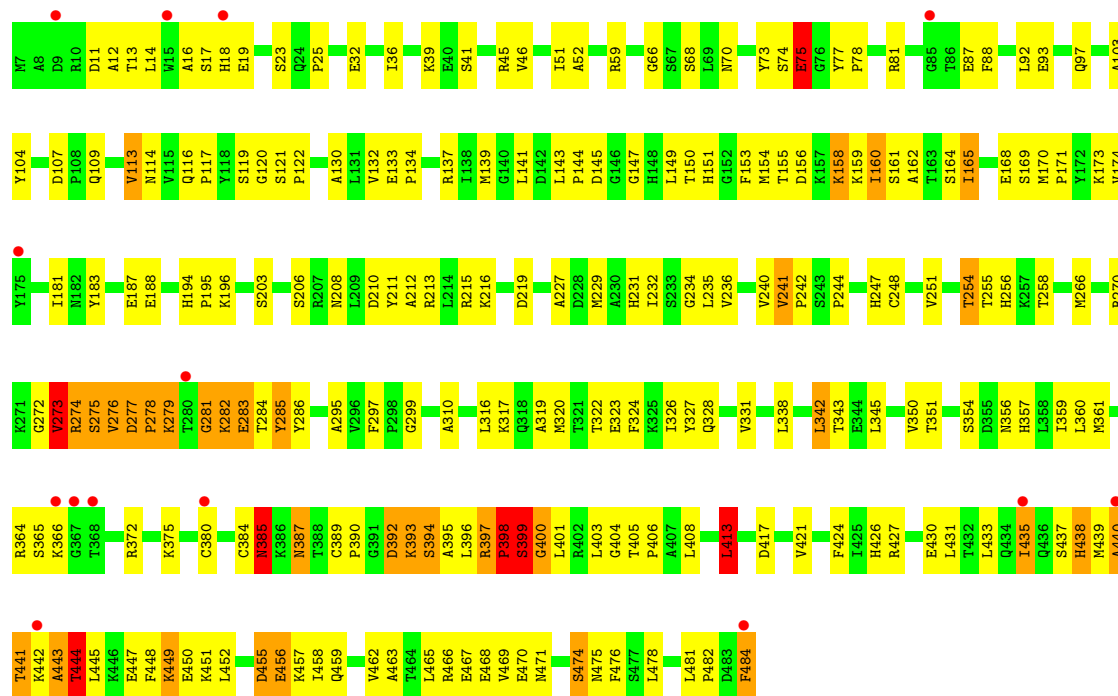


• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

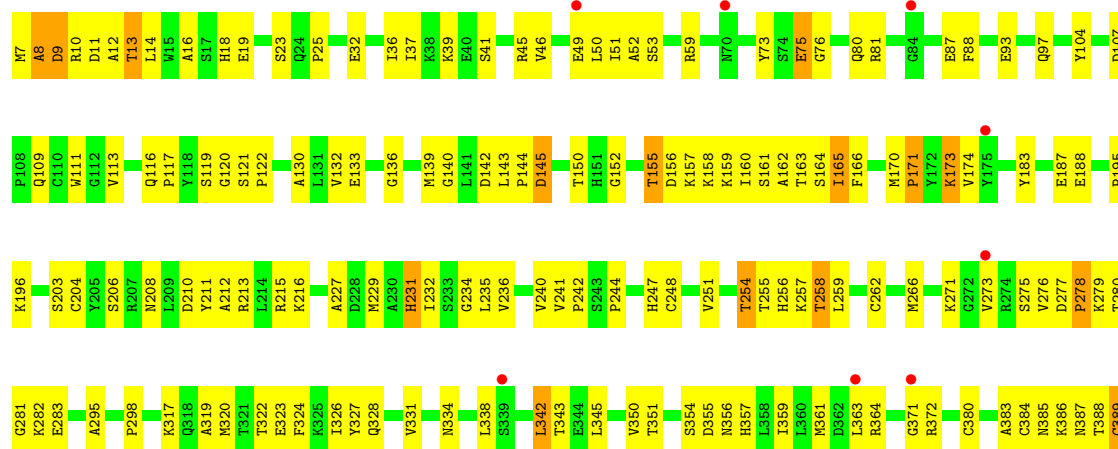


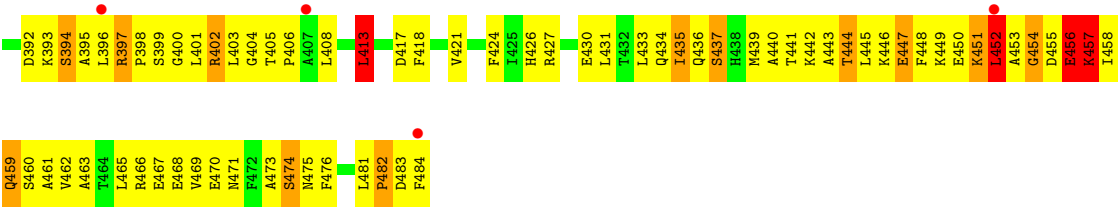


● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE



● Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	142.52Å 142.52Å 270.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.10 – 2.90 32.10 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.7 (32.10-2.90) 91.6 (32.10-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.90Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.271 , 0.228 0.265 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	75.1	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 81.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14984	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.52	2/3760 (0.1%)	0.99	12/5063 (0.2%)
1	B	0.53	1/3760 (0.0%)	1.00	11/5063 (0.2%)
1	C	0.51	1/3760 (0.0%)	1.02	19/5063 (0.4%)
1	D	0.48	0/3760	0.99	13/5063 (0.3%)
All	All	0.51	4/15040 (0.0%)	1.00	55/20252 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	387	ASN	CG-OD1	5.44	1.33	1.23
1	A	231	HIS	ND1-CE1	5.25	1.37	1.32
1	B	387	ASN	CG-OD1	5.21	1.33	1.23
1	A	387	ASN	CG-OD1	5.18	1.33	1.23

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	457	LYS	N-CA-C	-11.32	98.90	113.17
1	C	393	LYS	N-CA-C	-10.90	98.50	112.23
1	C	397	ARG	CA-C-N	8.34	130.27	119.84
1	C	397	ARG	C-N-CA	8.34	130.27	119.84
1	A	386	LYS	N-CA-C	-7.40	101.41	111.55
1	C	279	LYS	N-CA-C	-7.23	104.07	114.12
1	C	160	ILE	N-CA-C	6.85	116.97	110.74
1	C	151	HIS	N-CA-C	-6.74	105.03	112.72
1	D	173	LYS	N-CA-C	6.70	118.69	109.18
1	A	231	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	A	173	LYS	N-CA-C	6.38	118.23	109.18
1	C	173	LYS	N-CA-C	6.29	118.11	109.18
1	D	437	SER	N-CA-C	6.24	118.88	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	LYS	N-CA-C	-6.17	105.92	113.50
1	D	9	ASP	N-CA-C	-6.12	105.87	113.15
1	C	196	LYS	N-CA-C	-6.05	106.06	113.50
1	A	343	THR	N-CA-C	-6.01	104.64	111.14
1	C	203	SER	N-CA-C	-5.98	106.59	114.31
1	A	203	SER	N-CA-C	-5.97	106.61	114.31
1	D	459	GLN	N-CA-C	-5.96	98.10	110.80
1	C	343	THR	N-CA-C	-5.88	104.79	111.14
1	D	196	LYS	N-CA-C	-5.87	106.28	113.50
1	C	399	SER	CA-C-N	-5.84	115.34	121.35
1	C	399	SER	C-N-CA	-5.84	115.34	121.35
1	B	75	GLU	N-CA-C	5.80	123.15	110.80
1	B	343	THR	N-CA-C	-5.79	104.88	111.14
1	A	75	GLU	N-CA-C	5.79	123.13	110.80
1	D	343	THR	N-CA-C	-5.76	104.92	111.14
1	C	400	GLY	N-CA-C	5.70	119.46	110.96
1	D	75	GLU	N-CA-C	5.66	122.85	110.80
1	D	45	ARG	NE-CZ-NH2	5.65	124.28	119.20
1	B	196	LYS	N-CA-C	-5.65	106.56	113.50
1	C	158	LYS	N-CA-C	5.64	117.67	108.76
1	B	397	ARG	CA-C-N	5.62	126.87	119.84
1	B	397	ARG	C-N-CA	5.62	126.87	119.84
1	A	231	HIS	CB-CG-ND1	5.56	131.04	122.70
1	C	165	ILE	CB-CA-C	-5.56	104.76	112.04
1	D	165	ILE	CB-CA-C	-5.52	104.80	112.04
1	D	254	THR	N-CA-C	-5.46	102.45	110.52
1	B	439	MSE	N-CA-C	5.45	117.08	108.96
1	B	254	THR	N-CA-C	-5.45	101.97	110.42
1	D	355	ASP	N-CA-C	-5.45	106.64	113.72
1	A	45	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	355	ASP	N-CA-C	-5.40	106.70	113.72
1	B	203	SER	N-CA-C	-5.37	106.61	114.39
1	C	254	THR	N-CA-C	-5.35	102.12	110.42
1	D	203	SER	N-CA-C	-5.35	106.68	114.12
1	A	254	THR	N-CA-C	-5.34	102.14	110.42
1	B	419	GLN	N-CA-C	-5.31	105.16	111.69
1	C	241	VAL	CA-C-N	5.23	125.47	119.83
1	C	241	VAL	C-N-CA	5.23	125.47	119.83
1	D	45	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	B	285	TYR	N-CA-C	5.22	117.82	110.14
1	C	75	GLU	N-CA-C	5.08	121.63	110.80
1	A	158	LYS	N-CA-C	5.02	117.93	109.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3695	0	3660	184	0
1	B	3695	0	3660	198	0
1	C	3695	0	3658	224	0
1	D	3695	0	3658	215	0
2	A	20	0	11	1	0
2	B	20	0	11	5	0
2	C	20	0	10	3	0
2	D	20	0	10	2	0
3	A	34	0	21	3	0
3	B	34	0	21	1	0
3	D	34	0	21	1	0
4	A	5	0	0	1	0
4	B	4	0	0	0	0
4	C	9	0	0	2	0
4	D	4	0	0	1	0
All	All	14984	0	14741	781	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 26.

All (781) 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:155:THR:HG22	1:D:157:LYS:H	1.21	1.04
1:B:280:THR:HB	1:B:282:LYS:HE3	1.40	1.01
1:C:59:ARG:HG3	1:C:481:LEU:HD23	1.47	0.97
1:D:458:ILE:C	1:D:460:SER:H	1.67	0.97
1:A:435:ILE:HD12	1:A:448:PHE:HE1	1.30	0.94
1:A:432:THR:O	1:A:436:GLN:HG2	1.68	0.94
1:C:234:GLY:HA3	1:C:258:THR:O	1.67	0.92
1:C:155:THR:HG23	1:C:158:LYS:H	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:MET:N	1:D:10:ARG:HD3	1.89	0.87
1:C:384:CYS:O	1:C:385:ASN:HB2	1.74	0.87
1:D:452:LEU:HD13	1:D:453:ALA:H	1.40	0.87
1:C:361:MSE:HE2	1:C:403:LEU:HD11	1.57	0.87
1:C:276:VAL:HA	1:C:282:LYS:HB2	1.55	0.86
1:B:456:GLU:HB3	1:B:458:ILE:H	1.41	0.85
1:A:451:LYS:HB3	1:A:458:ILE:HD12	1.60	0.83
1:A:350:VAL:HG12	1:A:351:THR:HG23	1.61	0.83
1:B:456:GLU:CB	1:B:458:ILE:HG22	2.09	0.83
1:D:458:ILE:C	1:D:460:SER:N	2.31	0.82
1:D:155:THR:HG22	1:D:157:LYS:N	1.95	0.82
1:D:155:THR:CG2	1:D:157:LYS:H	1.92	0.82
1:C:276:VAL:HG13	1:C:281:GLY:HA2	1.62	0.81
1:C:275:SER:CB	1:C:284:THR:H	1.93	0.81
1:D:52:ALA:HB3	1:D:402:ARG:HH11	1.46	0.81
1:A:435:ILE:HD12	1:A:448:PHE:CE1	2.17	0.80
1:B:361:MSE:HE2	1:B:403:LEU:HD11	1.63	0.80
1:B:279:LYS:N	1:B:279:LYS:HD2	1.97	0.80
1:A:75:GLU:HG3	1:A:83:TYR:HE2	1.47	0.78
1:D:350:VAL:HG12	1:D:351:THR:HG23	1.63	0.78
1:B:453:ALA:C	1:B:455:ASP:H	1.90	0.78
1:C:277:ASP:HB3	1:C:278:PRO:HD3	1.66	0.78
1:C:372:ARG:NH2	1:C:443:ALA:HB1	1.99	0.77
1:C:398:PRO:O	1:C:399:SER:HB2	1.84	0.77
1:A:397:ARG:N	1:A:398:PRO:HD3	1.98	0.77
1:B:397:ARG:N	1:B:398:PRO:HD3	1.98	0.77
1:C:145:ASP:OD2	1:C:174:VAL:HG22	1.85	0.77
1:C:444:THR:HG22	1:C:447:GLU:H	1.47	0.76
1:D:435:ILE:HG13	1:D:452:LEU:HD23	1.66	0.76
1:B:143:LEU:C	1:B:143:LEU:HD23	2.10	0.76
1:A:361:MSE:HE2	1:A:403:LEU:HD11	1.65	0.76
1:D:361:MSE:HE2	1:D:403:LEU:HD11	1.67	0.75
1:C:159:LYS:HD3	1:C:164:SER:O	1.85	0.75
1:C:350:VAL:HG12	1:C:351:THR:HG23	1.67	0.75
1:D:208:ASN:ND2	1:D:242:PRO:HD2	2.02	0.75
1:D:435:ILE:O	1:D:435:ILE:HD13	1.87	0.75
1:B:372:ARG:HH12	1:B:397:ARG:NH1	1.85	0.74
1:A:120:GLY:HA3	2:A:500:PLG:H5A2	1.69	0.74
1:A:277:ASP:HB3	1:A:280:THR:HG23	1.67	0.74
1:A:387:ASN:HD21	3:A:600:THF:HN1	1.32	0.74
1:D:467:GLU:HG2	1:D:471:ASN:HD21	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LYS:HE2	1:A:458:ILE:HD11	1.68	0.73
1:B:389:CYS:HB2	1:B:390:PRO:HD2	1.69	0.73
1:D:322:THR:O	1:D:326:ILE:HG22	1.88	0.73
1:A:447:GLU:O	1:A:450:GLU:HG2	1.87	0.73
1:A:467:GLU:HG2	1:A:471:ASN:HD21	1.52	0.73
1:B:350:VAL:HG12	1:B:351:THR:HG23	1.70	0.73
1:A:386:LYS:O	1:A:398:PRO:HG2	1.88	0.73
1:C:208:ASN:ND2	1:C:242:PRO:HD2	2.03	0.73
1:B:208:ASN:ND2	1:B:242:PRO:HD2	2.03	0.73
1:B:456:GLU:HB3	1:B:458:ILE:HG22	1.69	0.73
1:D:452:LEU:HD13	1:D:453:ALA:N	2.02	0.73
1:D:46:VAL:HG12	1:D:474:SER:HB3	1.71	0.73
1:D:452:LEU:CD1	1:D:453:ALA:H	2.02	0.73
1:B:456:GLU:HB2	1:B:458:ILE:HG22	1.71	0.72
1:A:435:ILE:HD13	1:A:435:ILE:O	1.89	0.72
1:B:46:VAL:HG12	1:B:474:SER:HB3	1.71	0.72
1:B:387:ASN:HD21	3:B:601:THF:HN1	1.38	0.72
1:A:386:LYS:HE3	1:A:396:LEU:HA	1.71	0.72
1:B:380:CYS:SG	1:B:462:VAL:HG23	2.30	0.72
1:A:208:ASN:ND2	1:A:242:PRO:HD2	2.04	0.72
1:D:447:GLU:O	1:D:451:LYS:HE2	1.90	0.72
1:C:46:VAL:HG12	1:C:474:SER:HB3	1.72	0.71
1:C:459:GLN:HA	1:C:462:VAL:HG12	1.71	0.71
1:C:93:GLU:O	1:C:97:GLN:HG3	1.91	0.70
1:C:14:LEU:H	1:C:14:LEU:HD12	1.56	0.70
1:A:451:LYS:HE2	1:A:458:ILE:CD1	2.21	0.70
1:A:46:VAL:HG12	1:A:474:SER:HB3	1.72	0.70
1:B:444:THR:HG23	1:B:447:GLU:OE2	1.92	0.70
1:C:467:GLU:HG2	1:C:471:ASN:HD21	1.55	0.70
1:D:255:THR:HG22	1:D:266:MSE:HE2	1.74	0.70
1:A:380:CYS:SG	1:A:462:VAL:HG23	2.32	0.69
1:D:52:ALA:HB3	1:D:402:ARG:NH1	2.07	0.69
1:A:459:GLN:HA	1:A:462:VAL:HG12	1.72	0.69
1:B:158:LYS:HE3	1:B:160:ILE:CD1	2.22	0.69
1:B:322:THR:O	1:B:326:ILE:HG22	1.91	0.69
1:D:240:VAL:HG23	1:D:241:VAL:HG13	1.73	0.69
1:C:187:GLU:OE1	1:C:216:LYS:HE3	1.92	0.69
1:A:361:MSE:HE3	1:A:401:LEU:HB2	1.74	0.69
1:A:322:THR:O	1:A:326:ILE:HG22	1.93	0.69
1:D:7:MET:N	1:D:10:ARG:HH21	1.91	0.69
1:D:380:CYS:SG	1:D:462:VAL:HG23	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLU:O	1:A:97:GLN:HG3	1.92	0.68
1:B:235:LEU:HD23	1:B:328:GLN:HG3	1.76	0.68
1:C:443:ALA:O	1:C:444:THR:HB	1.94	0.68
1:C:282:LYS:O	1:C:283:GLU:HB2	1.93	0.68
1:B:274:ARG:O	1:B:284:THR:HB	1.94	0.68
1:D:327:TYR:O	1:D:331:VAL:HG23	1.94	0.68
1:A:240:VAL:HG23	1:A:241:VAL:HG13	1.75	0.68
1:A:8:ALA:O	1:A:9:ASP:HB2	1.94	0.67
1:A:277:ASP:HB2	1:A:282:LYS:H	1.59	0.67
1:B:435:ILE:HD13	1:B:435:ILE:C	2.19	0.67
1:D:37:ILE:HG22	1:D:484:PHE:O	1.95	0.67
1:D:143:LEU:HD11	3:D:602:THF:O4	1.95	0.67
1:B:454:GLY:HA2	1:B:459:GLN:OE1	1.94	0.67
1:B:467:GLU:HG2	1:B:471:ASN:HD21	1.58	0.67
1:C:441:THR:OG1	1:C:442:LYS:HE3	1.95	0.67
1:C:361:MSE:HE3	1:C:401:LEU:HB2	1.75	0.67
1:B:51:ILE:HG12	1:B:384:CYS:O	1.95	0.66
1:D:120:GLY:HA3	2:D:503:PLG:H5A2	1.77	0.66
1:D:397:ARG:HH21	1:D:397:ARG:HG3	1.60	0.66
1:B:435:ILE:HD13	1:B:435:ILE:O	1.94	0.66
1:C:130:ALA:HB2	1:C:295:ALA:HB2	1.76	0.66
1:C:322:THR:O	1:C:326:ILE:HG22	1.96	0.66
1:A:413:LEU:HD22	1:A:476:PHE:CE2	2.30	0.66
1:A:317:LYS:HA	1:A:320:MSE:HE3	1.77	0.66
1:B:277:ASP:C	1:B:279:LYS:H	2.04	0.66
1:B:317:LYS:HA	1:B:320:MSE:HE3	1.78	0.66
1:C:317:LYS:HA	1:C:320:MSE:HE3	1.78	0.66
1:B:144:PRO:HB3	1:B:393:LYS:HE2	1.78	0.65
1:C:120:GLY:HA3	2:C:502:PLG:H5A2	1.78	0.65
1:C:155:THR:HG22	1:C:158:LYS:O	1.95	0.65
1:D:395:ALA:C	1:D:397:ARG:H	2.03	0.65
1:D:386:LYS:HG3	1:D:386:LYS:O	1.95	0.65
1:B:93:GLU:O	1:B:97:GLN:HG3	1.95	0.65
1:C:14:LEU:H	1:C:14:LEU:CD1	2.08	0.65
1:C:235:LEU:HD23	1:C:328:GLN:HG3	1.78	0.65
1:D:467:GLU:HG2	1:D:471:ASN:ND2	2.12	0.65
1:A:467:GLU:HG2	1:A:471:ASN:ND2	2.11	0.65
1:C:327:TYR:O	1:C:331:VAL:HG23	1.97	0.65
1:C:380:CYS:SG	1:C:462:VAL:HG23	2.37	0.65
1:C:445:LEU:HD22	1:C:449:LYS:HE3	1.79	0.64
1:A:16:ALA:O	1:A:19:GLU:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:GLN:HA	1:B:462:VAL:HG12	1.79	0.64
1:B:274:ARG:HD3	1:B:286:TYR:CE1	2.32	0.64
1:C:278:PRO:C	1:C:279:LYS:HD3	2.22	0.64
1:D:277:ASP:CG	1:D:278:PRO:HD2	2.22	0.64
1:B:396:LEU:C	1:B:398:PRO:HD3	2.23	0.64
1:D:450:GLU:O	1:D:452:LEU:N	2.31	0.64
1:B:280:THR:HG22	1:B:281:GLY:H	1.63	0.64
1:C:154:MSE:HE2	1:C:164:SER:HB2	1.80	0.64
1:C:240:VAL:HG23	1:C:241:VAL:HG13	1.79	0.64
1:C:413:LEU:HD22	1:C:476:PHE:CE2	2.32	0.63
1:A:435:ILE:HD13	1:A:435:ILE:C	2.23	0.63
1:B:394:SER:HB2	1:B:397:ARG:O	1.98	0.63
1:D:317:LYS:HA	1:D:320:MSE:HE3	1.81	0.63
1:A:121:SER:HB2	1:A:122:PRO:HD3	1.80	0.63
1:A:139:MSE:HG3	1:A:195:PRO:HB3	1.80	0.63
1:B:413:LEU:HD22	1:B:476:PHE:CE2	2.33	0.63
1:D:276:VAL:HG12	1:D:283:GLU:HG2	1.80	0.63
1:C:455:ASP:O	1:C:457:LYS:N	2.32	0.62
1:D:277:ASP:HB3	1:D:280:THR:HB	1.79	0.62
1:A:255:THR:HG22	1:A:266:MSE:HE2	1.81	0.62
1:C:278:PRO:HG2	1:C:282:LYS:HE3	1.81	0.62
1:C:449:LYS:HB2	1:C:449:LYS:NZ	2.14	0.62
1:D:51:ILE:HG13	1:D:383:ALA:HB1	1.81	0.62
1:B:148:HIS:HB2	1:B:203:SER:OG	1.99	0.62
1:B:385:ASN:C	1:B:385:ASN:HD22	2.07	0.62
1:D:212:ALA:HA	1:D:247:HIS:CD2	2.35	0.62
1:B:274:ARG:HB3	1:B:286:TYR:CE2	2.34	0.62
1:B:240:VAL:HG23	1:B:241:VAL:HG13	1.81	0.62
1:B:389:CYS:HB2	1:B:390:PRO:CD	2.29	0.62
1:B:453:ALA:O	1:B:455:ASP:N	2.32	0.62
1:C:121:SER:HB2	1:C:122:PRO:HD3	1.81	0.62
1:D:361:MSE:HE3	1:D:401:LEU:HB2	1.81	0.62
1:A:322:THR:HG22	1:B:14:LEU:HD21	1.80	0.62
1:C:322:THR:HG22	1:D:14:LEU:HD11	1.80	0.61
1:C:467:GLU:HG2	1:C:471:ASN:ND2	2.14	0.61
1:C:361:MSE:O	1:C:400:GLY:HA2	2.00	0.61
1:C:16:ALA:O	1:C:19:GLU:HB3	2.00	0.61
1:A:439:MSE:O	1:A:441:THR:HG23	2.01	0.61
1:D:16:ALA:O	1:D:19:GLU:HB3	2.00	0.61
1:B:121:SER:HB2	1:B:122:PRO:HD3	1.80	0.61
1:D:371:GLY:HA2	1:D:386:LYS:HD3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:ASP:O	1:D:456:GLU:C	2.43	0.61
1:D:459:GLN:HA	1:D:462:VAL:HG12	1.83	0.61
1:D:144:PRO:HA	1:D:388:THR:HG21	1.83	0.60
1:C:372:ARG:HH22	1:C:443:ALA:HB1	1.64	0.60
1:C:77:TYR:CE2	1:C:116:GLN:NE2	2.69	0.60
1:C:447:GLU:HA	1:C:447:GLU:OE1	2.01	0.60
1:D:395:ALA:O	1:D:396:LEU:HB2	2.01	0.60
1:B:148:HIS:HE1	1:B:150:THR:HG23	1.66	0.60
1:B:453:ALA:C	1:B:455:ASP:N	2.57	0.60
1:B:384:CYS:O	1:B:385:ASN:HB2	2.01	0.60
1:D:466:ARG:O	1:D:470:GLU:HG3	2.01	0.60
1:A:327:TYR:O	1:A:331:VAL:HG23	2.02	0.60
1:B:327:TYR:O	1:B:331:VAL:HG23	2.01	0.60
1:B:431:LEU:HD23	1:B:431:LEU:O	2.01	0.60
1:D:121:SER:HB2	1:D:122:PRO:HD3	1.83	0.60
1:B:467:GLU:HG2	1:B:471:ASN:ND2	2.16	0.60
1:B:361:MSE:HE3	1:B:401:LEU:HB2	1.84	0.60
1:A:437:SER:C	1:A:439:MSE:H	2.10	0.60
1:C:255:THR:HG22	1:C:266:MSE:HE2	1.84	0.60
1:C:435:ILE:HD13	1:C:435:ILE:O	2.02	0.60
1:B:158:LYS:HE3	1:B:160:ILE:HD11	1.84	0.59
1:C:278:PRO:HD2	1:C:282:LYS:HG3	1.82	0.59
1:D:364:ARG:NH2	1:D:392:ASP:OD2	2.35	0.59
1:B:435:ILE:HD12	1:B:448:PHE:CE1	2.36	0.59
1:D:93:GLU:O	1:D:97:GLN:HG3	2.02	0.59
1:B:280:THR:CB	1:B:282:LYS:HE3	2.25	0.59
1:C:361:MSE:HE3	1:C:401:LEU:HD12	1.85	0.59
1:C:345:LEU:HD13	1:C:426:HIS:HB2	1.84	0.59
1:D:435:ILE:HD13	1:D:435:ILE:C	2.26	0.59
1:B:16:ALA:O	1:B:19:GLU:HB3	2.01	0.59
1:A:413:LEU:HD22	1:A:476:PHE:CD2	2.37	0.59
1:B:446:LYS:O	1:B:450:GLU:HG2	2.02	0.59
1:C:278:PRO:CG	1:C:282:LYS:HE3	2.32	0.59
1:D:111:TRP:C	1:D:271:LYS:HD3	2.28	0.59
1:D:121:SER:HA	1:D:150:THR:HG21	1.84	0.59
1:C:413:LEU:HD22	1:C:476:PHE:CD2	2.37	0.59
1:D:456:GLU:OE1	1:D:456:GLU:O	2.20	0.59
1:C:149:LEU:HD11	1:D:298:PRO:HB2	1.85	0.58
1:D:345:LEU:HD13	1:D:426:HIS:HB2	1.85	0.58
1:A:235:LEU:HD23	1:A:328:GLN:HG3	1.85	0.58
1:A:59:ARG:NH2	1:B:25:PRO:HG3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ARG:HG3	1:C:213:ARG:HH11	1.68	0.58
1:D:405:THR:H	1:D:406:PRO:HD3	1.69	0.58
1:B:345:LEU:HD13	1:B:426:HIS:HB2	1.85	0.58
1:A:431:LEU:HD23	1:A:431:LEU:O	2.03	0.58
1:A:462:VAL:HG13	1:A:463:ALA:N	2.19	0.58
1:C:440:ALA:O	1:C:441:THR:HG23	2.03	0.58
1:A:345:LEU:HD13	1:A:426:HIS:HB2	1.84	0.58
1:C:155:THR:CG2	1:C:158:LYS:H	2.13	0.58
1:C:273:VAL:O	1:C:285:TYR:HA	2.04	0.58
1:C:394:SER:HB3	1:C:397:ARG:O	2.04	0.58
1:C:361:MSE:CE	1:C:401:LEU:HD12	2.34	0.58
1:D:397:ARG:N	1:D:398:PRO:HD3	2.19	0.58
1:D:413:LEU:HD22	1:D:476:PHE:CE2	2.39	0.57
1:A:206:SER:HA	1:A:356:ASN:HD21	1.69	0.57
1:C:444:THR:HG22	1:C:447:GLU:N	2.18	0.57
1:D:143:LEU:HB3	1:D:144:PRO:HD3	1.86	0.57
1:B:431:LEU:O	1:B:435:ILE:HG22	2.05	0.57
1:C:11:ASP:O	1:C:13:THR:N	2.36	0.57
1:C:439:MSE:O	1:C:440:ALA:C	2.46	0.57
1:D:361:MSE:O	1:D:400:GLY:HA2	2.05	0.57
1:B:280:THR:HG22	1:B:281:GLY:N	2.18	0.57
1:C:326:ILE:HD13	1:D:14:LEU:HB3	1.86	0.57
1:D:49:GLU:HA	1:D:383:ALA:HB3	1.86	0.57
1:D:442:LYS:O	1:D:442:LYS:HG2	2.04	0.57
1:D:450:GLU:O	1:D:454:GLY:N	2.36	0.57
1:B:439:MSE:HE3	1:B:443:ALA:CB	2.34	0.57
1:D:50:LEU:HB2	1:D:383:ALA:O	2.05	0.57
1:C:75:GLU:HG2	1:C:297:PHE:CZ	2.39	0.57
1:C:459:GLN:HA	1:C:462:VAL:CG1	2.35	0.57
1:D:187:GLU:OE1	1:D:216:LYS:HE3	2.04	0.57
1:A:387:ASN:ND2	3:A:600:THF:HN1	2.00	0.56
1:B:256:HIS:O	1:B:257:LYS:HB2	2.03	0.56
1:D:10:ARG:C	1:D:12:ALA:H	2.13	0.56
1:C:59:ARG:HG3	1:C:481:LEU:CD2	2.29	0.56
1:C:143:LEU:HB3	1:C:144:PRO:CD	2.35	0.56
1:A:10:ARG:HB2	1:A:10:ARG:CZ	2.35	0.56
1:B:234:GLY:HA3	1:B:258:THR:O	2.05	0.56
1:B:413:LEU:HD22	1:B:476:PHE:CD2	2.40	0.56
1:D:161:SER:O	1:D:165:ILE:HG13	2.05	0.56
1:A:372:ARG:HD3	1:A:436:GLN:OE1	2.05	0.56
1:B:153:PHE:HD2	1:B:160:ILE:HB	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:THR:H	1:A:406:PRO:HD3	1.70	0.56
1:B:277:ASP:O	1:B:279:LYS:N	2.36	0.56
1:C:18:HIS:HB2	1:D:323:GLU:HB3	1.86	0.56
1:C:427:ARG:O	1:C:430:GLU:HB3	2.06	0.56
1:A:212:ALA:HA	1:A:247:HIS:CD2	2.41	0.56
1:B:162:ALA:HA	1:B:165:ILE:HD12	1.87	0.56
1:D:158:LYS:HD2	1:D:160:ILE:HD13	1.86	0.56
1:B:212:ALA:HA	1:B:247:HIS:CD2	2.41	0.56
1:C:212:ALA:HA	1:C:247:HIS:CD2	2.41	0.55
1:A:187:GLU:OE1	1:A:216:LYS:HE3	2.06	0.55
1:A:395:ALA:O	1:A:396:LEU:HB2	2.07	0.55
1:C:405:THR:H	1:C:406:PRO:HD3	1.70	0.55
1:C:466:ARG:O	1:C:470:GLU:HG3	2.06	0.55
1:D:235:LEU:HD23	1:D:328:GLN:HG3	1.88	0.55
1:A:141:LEU:O	1:A:147:GLY:HA3	2.05	0.55
1:D:50:LEU:H	1:D:383:ALA:HB3	1.72	0.55
1:D:51:ILE:HG12	1:D:384:CYS:O	2.06	0.55
1:A:386:LYS:CE	1:A:396:LEU:HA	2.35	0.55
1:B:139:MSE:HG3	1:B:195:PRO:HB3	1.89	0.55
1:D:458:ILE:HG22	1:D:461:ALA:HB2	1.89	0.55
1:D:139:MSE:HG3	1:D:195:PRO:HB3	1.87	0.55
1:B:159:LYS:HD3	1:B:164:SER:O	2.07	0.55
1:C:14:LEU:HD12	1:C:14:LEU:N	2.22	0.55
1:C:275:SER:HB2	1:C:284:THR:HB	1.89	0.55
1:D:363:LEU:HD21	1:D:401:LEU:HD11	1.88	0.55
1:D:413:LEU:HD22	1:D:476:PHE:CD2	2.42	0.55
1:B:466:ARG:O	1:B:470:GLU:HG3	2.07	0.55
1:B:104:TYR:CZ	1:B:229:MSE:HE1	2.43	0.54
1:C:143:LEU:HB3	1:C:144:PRO:HD3	1.88	0.54
1:D:41:SER:HB2	1:D:484:PHE:O	2.07	0.54
1:D:427:ARG:O	1:D:430:GLU:HB3	2.07	0.54
1:A:274:ARG:HB3	1:A:284:THR:O	2.07	0.54
1:A:450:GLU:C	1:A:452:LEU:N	2.65	0.54
1:C:375:LYS:HG2	1:C:449:LYS:HG2	1.89	0.54
1:C:435:ILE:HD13	1:C:435:ILE:C	2.32	0.54
1:B:374:GLU:OE1	1:B:386:LYS:N	2.40	0.54
1:C:277:ASP:O	1:C:278:PRO:O	2.26	0.54
1:D:213:ARG:HG3	1:D:213:ARG:HH11	1.71	0.54
1:D:338:LEU:O	1:D:342:LEU:HB2	2.07	0.54
1:D:393:LYS:O	1:D:394:SER:HB3	2.05	0.54
1:A:323:GLU:HB3	1:B:18:HIS:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:VAL:HG13	1:B:463:ALA:N	2.21	0.54
1:C:394:SER:O	1:C:395:ALA:HB3	2.08	0.54
1:A:66:GLY:O	1:B:481:LEU:HD11	2.08	0.54
1:C:405:THR:N	1:C:406:PRO:CD	2.71	0.54
1:A:215:ARG:HG3	1:A:247:HIS:HB3	1.89	0.54
1:A:405:THR:N	1:A:406:PRO:CD	2.71	0.54
1:A:451:LYS:HA	1:A:455:ASP:HB2	1.89	0.54
1:A:466:ARG:O	1:A:470:GLU:HG3	2.08	0.54
1:D:450:GLU:C	1:D:452:LEU:N	2.66	0.54
1:D:462:VAL:HG13	1:D:463:ALA:N	2.21	0.54
1:A:431:LEU:O	1:A:435:ILE:HG22	2.07	0.53
1:A:277:ASP:CB	1:A:280:THR:HG23	2.36	0.53
1:A:438:HIS:O	1:A:451:LYS:NZ	2.40	0.53
1:C:462:VAL:HG13	1:C:463:ALA:N	2.23	0.53
1:B:255:THR:HG22	1:B:266:MSE:HE2	1.89	0.53
1:C:338:LEU:O	1:C:342:LEU:HB2	2.08	0.53
1:A:213:ARG:HG3	1:A:213:ARG:HH11	1.71	0.53
1:B:427:ARG:O	1:B:430:GLU:HB3	2.08	0.53
1:C:104:TYR:CZ	1:C:229:MSE:HE1	2.43	0.53
1:D:471:ASN:O	1:D:475:ASN:ND2	2.41	0.53
1:C:14:LEU:HD23	1:D:322:THR:HG22	1.89	0.53
1:C:235:LEU:HD23	1:C:328:GLN:CG	2.38	0.53
1:D:457:LYS:HE3	1:D:457:LYS:HA	1.90	0.53
1:C:456:GLU:O	1:C:457:LYS:C	2.52	0.53
1:B:395:ALA:C	1:B:397:ARG:H	2.16	0.53
1:B:405:THR:H	1:B:406:PRO:HD3	1.72	0.53
1:D:215:ARG:HG3	1:D:247:HIS:HB3	1.90	0.53
1:D:431:LEU:HD23	1:D:431:LEU:O	2.08	0.53
1:A:338:LEU:O	1:A:342:LEU:HB2	2.09	0.53
1:C:439:MSE:O	1:C:440:ALA:O	2.27	0.53
1:D:405:THR:N	1:D:406:PRO:CD	2.72	0.53
1:B:431:LEU:HD23	1:B:431:LEU:C	2.33	0.53
1:C:154:MSE:HE1	4:C:527:HOH:O	2.09	0.53
1:C:398:PRO:O	1:C:399:SER:CB	2.57	0.53
1:A:10:ARG:HB2	1:A:10:ARG:NH2	2.24	0.52
1:C:433:LEU:O	1:C:437:SER:N	2.41	0.52
1:D:232:ILE:O	1:D:236:VAL:HG23	2.09	0.52
1:B:257:LYS:HZ1	2:B:501:PLG:C4A	2.22	0.52
1:B:393:LYS:O	1:B:393:LYS:HG3	2.09	0.52
1:D:431:LEU:O	1:D:435:ILE:HG22	2.09	0.52
1:A:10:ARG:NH1	1:B:414:LEU:HD11	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PHE:HE1	1:A:468:GLU:HG2	1.74	0.52
1:A:450:GLU:C	1:A:452:LEU:H	2.16	0.52
1:B:143:LEU:C	1:B:143:LEU:CD2	2.82	0.52
1:D:405:THR:N	1:D:406:PRO:HD3	2.25	0.52
1:B:279:LYS:N	1:B:279:LYS:CD	2.69	0.52
1:C:74:SER:HB2	1:C:81:ARG:NH1	2.25	0.52
1:C:275:SER:CB	1:C:284:THR:N	2.69	0.52
1:D:130:ALA:HB2	1:D:295:ALA:HB2	1.91	0.52
1:A:107:ASP:OD2	1:A:109:GLN:HB2	2.10	0.52
1:B:405:THR:N	1:B:406:PRO:CD	2.73	0.52
1:A:256:HIS:O	1:A:257:LYS:HB2	2.10	0.52
1:B:338:LEU:O	1:B:342:LEU:HB2	2.10	0.52
1:B:455:ASP:O	1:B:456:GLU:CB	2.58	0.52
1:D:456:GLU:OE1	1:D:458:ILE:N	2.36	0.52
1:C:141:LEU:O	1:C:147:GLY:HA3	2.10	0.52
1:B:104:TYR:CE2	1:B:229:MSE:HE1	2.44	0.51
1:D:143:LEU:HB3	1:D:144:PRO:CD	2.39	0.51
1:C:392:ASP:OD2	1:C:399:SER:HB2	2.10	0.51
1:D:445:LEU:HD11	1:D:446:LYS:HE3	1.91	0.51
1:A:481:LEU:HB3	1:A:482:PRO:CD	2.40	0.51
1:B:357:HIS:HD1	1:B:357:HIS:H	1.57	0.51
1:C:153:PHE:HD2	1:C:160:ILE:HB	1.75	0.51
1:A:431:LEU:HD23	1:A:431:LEU:C	2.35	0.51
1:C:41:SER:HB2	1:C:484:PHE:O	2.10	0.51
1:B:9:ASP:O	1:B:11:ASP:N	2.42	0.51
1:B:277:ASP:N	1:B:278:PRO:HD3	2.26	0.51
1:C:130:ALA:HB2	1:C:295:ALA:CB	2.40	0.51
1:A:427:ARG:O	1:A:430:GLU:HB3	2.11	0.51
1:C:32:GLU:O	1:C:36:ILE:HG13	2.11	0.51
1:C:275:SER:O	1:C:276:VAL:O	2.29	0.51
1:D:159:LYS:HD3	1:D:164:SER:O	2.10	0.51
1:D:206:SER:HA	1:D:356:ASN:HD21	1.76	0.51
1:A:385:ASN:OD1	1:A:402:ARG:NH2	2.39	0.51
1:A:413:LEU:HD13	1:A:417:ASP:HB3	1.92	0.51
1:B:213:ARG:HH11	1:B:213:ARG:HG3	1.75	0.51
1:C:254:THR:HB	1:C:256:HIS:CE1	2.46	0.51
1:A:77:TYR:C	1:A:79:GLY:N	2.69	0.50
1:B:32:GLU:O	1:B:36:ILE:HG13	2.10	0.50
1:D:439:MSE:HE2	1:D:443:ALA:CB	2.40	0.50
1:A:154:MSE:HE3	1:A:159:LYS:HG2	1.93	0.50
1:B:206:SER:HA	1:B:356:ASN:HD21	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:SER:HB2	1:C:81:ARG:HH11	1.76	0.50
1:C:274:ARG:HG2	1:C:286:TYR:OH	2.10	0.50
1:C:431:LEU:O	1:C:435:ILE:HG22	2.11	0.50
1:A:204:CYS:SG	1:A:387:ASN:OD1	2.64	0.50
1:C:471:ASN:O	1:C:475:ASN:ND2	2.45	0.50
1:A:232:ILE:O	1:A:236:VAL:HG23	2.11	0.50
1:B:235:LEU:HD23	1:B:328:GLN:CG	2.40	0.50
1:B:413:LEU:HD13	1:B:417:ASP:HB3	1.91	0.50
1:D:231:HIS:HD2	1:D:357:HIS:NE2	2.09	0.50
1:D:413:LEU:HD13	1:D:417:ASP:HB3	1.93	0.50
1:C:104:TYR:CE2	1:C:229:MSE:HE1	2.47	0.50
1:D:395:ALA:C	1:D:397:ARG:N	2.70	0.50
1:D:450:GLU:O	1:D:454:GLY:HA3	2.12	0.50
1:D:459:GLN:CA	1:D:462:VAL:HG12	2.42	0.50
1:D:444:THR:HG23	1:D:447:GLU:CD	2.36	0.50
1:A:211:TYR:CZ	1:A:244:PRO:HB3	2.46	0.50
1:A:389:CYS:O	1:A:391:GLY:N	2.44	0.50
1:C:139:MSE:HG3	1:C:195:PRO:HB3	1.93	0.50
1:B:254:THR:HB	1:B:256:HIS:CE1	2.47	0.49
1:C:282:LYS:O	1:C:283:GLU:CB	2.60	0.49
1:B:452:LEU:HD13	1:B:452:LEU:O	2.11	0.49
1:A:7:MET:C	1:A:9:ASP:H	2.19	0.49
1:C:405:THR:N	1:C:406:PRO:HD3	2.27	0.49
1:C:431:LEU:O	1:C:431:LEU:HD23	2.12	0.49
1:C:393:LYS:O	1:C:394:SER:C	2.55	0.49
1:D:9:ASP:O	1:D:13:THR:HB	2.13	0.49
1:A:442:LYS:O	1:A:442:LYS:HG2	2.13	0.49
1:C:215:ARG:HG3	1:C:247:HIS:HB3	1.93	0.49
1:C:274:ARG:HG2	1:C:274:ARG:HH11	1.76	0.49
1:C:323:GLU:HA	1:D:14:LEU:HD12	1.94	0.49
1:D:424:PHE:HE1	1:D:468:GLU:HG2	1.76	0.49
1:A:374:GLU:OE1	1:A:386:LYS:N	2.45	0.49
1:A:424:PHE:CE1	1:A:468:GLU:HG2	2.47	0.49
1:C:273:VAL:HG12	1:C:274:ARG:N	2.28	0.49
1:D:424:PHE:CE1	1:D:468:GLU:HG2	2.47	0.49
1:B:277:ASP:C	1:B:279:LYS:N	2.71	0.49
1:D:162:ALA:HA	1:D:165:ILE:HD12	1.95	0.49
1:D:396:LEU:C	1:D:398:PRO:HD3	2.37	0.49
1:B:384:CYS:O	1:B:385:ASN:CB	2.60	0.49
1:C:413:LEU:HD13	1:C:417:ASP:HB3	1.95	0.49
1:A:10:ARG:C	1:A:12:ALA:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:THR:HG22	4:D:526:HOH:O	2.13	0.49
1:B:449:LYS:NZ	1:B:449:LYS:HB2	2.28	0.48
1:C:206:SER:HA	1:C:356:ASN:HD21	1.78	0.48
1:D:384:CYS:HB3	1:D:385:ASN:H	1.50	0.48
1:A:11:ASP:O	1:A:12:ALA:C	2.55	0.48
1:C:215:ARG:HH11	1:C:219:ASP:CG	2.21	0.48
1:D:450:GLU:O	1:D:451:LYS:C	2.56	0.48
1:A:25:PRO:HG3	1:B:59:ARG:NH2	2.28	0.48
1:B:119:SER:C	1:B:122:PRO:HD2	2.39	0.48
1:C:396:LEU:C	1:C:398:PRO:HD3	2.38	0.48
1:D:389:CYS:N	1:D:392:ASP:OD1	2.45	0.48
1:C:107:ASP:OD2	1:C:109:GLN:HB2	2.13	0.48
1:D:227:ALA:HB2	1:D:248:CYS:SG	2.54	0.48
1:B:132:VAL:O	1:B:133:GLU:HB2	2.13	0.48
1:B:397:ARG:N	1:B:398:PRO:CD	2.71	0.48
1:D:107:ASP:OD2	1:D:109:GLN:HB2	2.13	0.48
1:A:437:SER:C	1:A:439:MSE:N	2.72	0.48
1:C:392:ASP:HB2	1:C:394:SER:OG	2.14	0.48
1:D:397:ARG:HG3	1:D:397:ARG:NH2	2.26	0.48
1:B:187:GLU:OE1	1:B:216:LYS:HE3	2.14	0.48
1:D:441:THR:C	1:D:443:ALA:H	2.22	0.48
1:C:77:TYR:CD2	1:C:116:GLN:NE2	2.81	0.48
1:C:235:LEU:CD2	1:C:328:GLN:HG3	2.44	0.48
1:C:424:PHE:HE1	1:C:468:GLU:HG2	1.78	0.48
1:D:385:ASN:HB2	1:D:402:ARG:HB3	1.94	0.48
1:A:59:ARG:HG3	1:A:481:LEU:HD23	1.95	0.48
1:A:471:ASN:O	1:A:475:ASN:ND2	2.46	0.48
1:B:263:ARG:HG2	1:B:263:ARG:HH11	1.78	0.48
1:A:18:HIS:CD2	1:B:327:TYR:HB2	2.48	0.48
1:C:417:ASP:O	1:C:421:VAL:HG23	2.13	0.48
1:D:204:CYS:SG	1:D:387:ASN:ND2	2.87	0.48
1:D:357:HIS:HD1	1:D:357:HIS:H	1.62	0.48
1:D:431:LEU:HD23	1:D:431:LEU:C	2.39	0.48
1:A:234:GLY:HA3	1:A:258:THR:O	2.14	0.47
1:B:148:HIS:CE1	1:B:150:THR:H	2.32	0.47
1:B:361:MSE:O	1:B:400:GLY:HA2	2.13	0.47
1:D:119:SER:C	1:D:122:PRO:HD2	2.39	0.47
1:A:326:ILE:HG21	1:B:14:LEU:HD23	1.95	0.47
1:A:450:GLU:O	1:A:452:LEU:N	2.47	0.47
1:C:66:GLY:O	1:D:481:LEU:CD1	2.62	0.47
1:C:270:ARG:NH1	1:C:274:ARG:NH1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLU:O	1:D:36:ILE:HG13	2.14	0.47
1:A:51:ILE:HG12	1:A:384:CYS:HA	1.96	0.47
1:C:275:SER:HB3	1:C:284:THR:H	1.74	0.47
1:C:365:SER:O	1:C:366:LYS:HG2	2.13	0.47
1:B:11:ASP:C	1:B:13:THR:H	2.22	0.47
1:B:14:LEU:O	1:B:17:SER:N	2.47	0.47
1:D:447:GLU:N	1:D:447:GLU:OE2	2.46	0.47
1:A:119:SER:C	1:A:122:PRO:HD2	2.38	0.47
1:B:439:MSE:HE3	1:B:443:ALA:HB1	1.96	0.47
1:C:213:ARG:HH11	1:C:213:ARG:CG	2.26	0.47
1:D:445:LEU:O	1:D:449:LYS:HB2	2.14	0.47
1:A:366:LYS:O	1:A:433:LEU:HD11	2.15	0.47
1:A:405:THR:N	1:A:406:PRO:HD3	2.29	0.47
1:A:445:LEU:HD13	1:A:445:LEU:H	1.80	0.47
1:C:319:ALA:HA	1:C:324:PHE:CG	2.50	0.47
1:C:424:PHE:CE1	1:C:468:GLU:HG2	2.50	0.47
1:D:104:TYR:CE2	1:D:229:MSE:HE1	2.50	0.47
1:B:211:TYR:CZ	1:B:244:PRO:HB3	2.49	0.47
1:B:471:ASN:O	1:B:475:ASN:ND2	2.48	0.47
1:C:270:ARG:HH12	1:C:274:ARG:HD3	1.80	0.47
1:D:116:GLN:N	1:D:117:PRO:CD	2.77	0.47
1:D:465:LEU:O	1:D:469:VAL:HG23	2.15	0.47
1:B:215:ARG:HG3	1:B:247:HIS:HB3	1.95	0.47
1:C:25:PRO:HG3	1:D:59:ARG:NH2	2.30	0.47
1:C:455:ASP:OD2	1:C:458:ILE:HG13	2.14	0.47
1:A:263:ARG:NH1	4:A:510:HOH:O	2.45	0.47
1:B:459:GLN:HA	1:B:462:VAL:CG1	2.45	0.47
1:D:235:LEU:HD23	1:D:328:GLN:CG	2.45	0.47
1:D:235:LEU:HD23	1:D:328:GLN:NE2	2.30	0.47
1:D:281:GLY:O	1:D:283:GLU:HG3	2.14	0.47
1:C:23:SER:O	1:D:59:ARG:HD3	2.15	0.46
1:D:208:ASN:HD22	1:D:242:PRO:HD2	1.76	0.46
1:D:279:LYS:O	1:D:279:LYS:HG2	2.14	0.46
1:A:145:ASP:OD2	1:A:174:VAL:HG22	2.16	0.46
1:A:388:THR:HA	1:A:398:PRO:HB3	1.98	0.46
1:B:447:GLU:HA	1:B:450:GLU:CG	2.45	0.46
1:C:78:PRO:HG3	1:C:81:ARG:HH21	1.80	0.46
1:D:80:GLN:HG3	1:D:80:GLN:O	2.14	0.46
1:A:104:TYR:CZ	1:A:229:MSE:HE1	2.50	0.46
1:C:51:ILE:HA	4:C:525:HOH:O	2.15	0.46
1:C:459:GLN:CA	1:C:462:VAL:HG12	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ARG:N	1:A:398:PRO:CD	2.74	0.46
1:C:174:VAL:HG21	1:C:390:PRO:HG3	1.98	0.46
1:D:433:LEU:O	1:D:437:SER:N	2.44	0.46
1:B:143:LEU:HD23	1:B:143:LEU:O	2.14	0.46
1:B:385:ASN:C	1:B:385:ASN:ND2	2.73	0.46
1:C:235:LEU:HD23	1:C:328:GLN:NE2	2.31	0.46
1:D:227:ALA:HB3	1:D:251:VAL:HG22	1.98	0.46
1:D:364:ARG:HB2	1:D:399:SER:HB3	1.97	0.46
1:A:235:LEU:HD23	1:A:328:GLN:NE2	2.30	0.46
1:D:211:TYR:CZ	1:D:244:PRO:HB3	2.50	0.46
1:D:213:ARG:HH11	1:D:213:ARG:CG	2.28	0.46
1:A:395:ALA:O	1:A:396:LEU:CB	2.62	0.46
1:D:8:ALA:C	1:D:10:ARG:H	2.23	0.46
1:D:393:LYS:O	1:D:394:SER:CB	2.63	0.46
1:B:274:ARG:HB3	1:B:286:TYR:CZ	2.50	0.46
1:C:275:SER:OG	1:C:276:VAL:N	2.47	0.46
1:A:116:GLN:N	1:A:117:PRO:CD	2.79	0.46
1:C:132:VAL:O	1:C:133:GLU:HB2	2.15	0.46
1:C:155:THR:HG23	1:C:158:LYS:N	2.16	0.46
1:A:275:SER:HB3	1:A:284:THR:OG1	2.17	0.45
1:B:200:ALA:HB2	1:B:214:LEU:HD13	1.98	0.45
1:B:424:PHE:HE1	1:B:468:GLU:HG2	1.80	0.45
1:D:10:ARG:CZ	1:D:10:ARG:HB3	2.45	0.45
1:D:104:TYR:CZ	1:D:229:MSE:HE1	2.51	0.45
1:D:481:LEU:O	1:D:483:ASP:N	2.48	0.45
1:A:323:GLU:OE1	1:A:323:GLU:N	2.45	0.45
1:B:183:TYR:CE2	1:B:210:ASP:HB3	2.50	0.45
1:B:263:ARG:HG2	1:B:263:ARG:NH1	2.31	0.45
1:C:14:LEU:O	1:C:17:SER:N	2.50	0.45
1:B:436:GLN:O	1:B:437:SER:C	2.59	0.45
1:C:59:ARG:NH2	1:D:25:PRO:HG3	2.31	0.45
1:B:280:THR:O	1:B:282:LYS:N	2.47	0.45
1:D:155:THR:CG2	1:D:156:ASP:N	2.78	0.45
1:A:207:ARG:NH1	1:A:355:ASP:OD2	2.48	0.45
1:A:361:MSE:O	1:A:400:GLY:HA2	2.16	0.45
1:C:119:SER:C	1:C:122:PRO:HD2	2.42	0.45
1:C:232:ILE:O	1:C:236:VAL:HG23	2.17	0.45
1:A:39:LYS:HB3	1:B:88:PHE:CE1	2.52	0.45
1:A:272:GLY:O	1:A:274:ARG:N	2.49	0.45
1:A:327:TYR:HB2	1:B:18:HIS:CD2	2.52	0.45
1:B:52:ALA:HA	1:B:404:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:THR:N	1:B:406:PRO:HD3	2.30	0.45
1:D:234:GLY:HA3	1:D:258:THR:O	2.17	0.45
1:D:439:MSE:HE2	1:D:443:ALA:HB1	1.97	0.45
1:A:302:GLY:HA3	2:B:501:PLG:OP1	2.16	0.45
1:B:391:GLY:O	1:B:392:ASP:HB2	2.17	0.45
1:D:277:ASP:CB	1:D:280:THR:HB	2.46	0.45
1:A:227:ALA:HB2	1:A:248:CYS:SG	2.57	0.45
1:C:70:ASN:HD21	1:D:262:CYS:HA	1.81	0.45
1:C:413:LEU:CD2	1:C:413:LEU:H	2.30	0.45
1:D:372:ARG:HG3	1:D:372:ARG:HH11	1.81	0.45
1:A:59:ARG:CZ	1:B:25:PRO:HG3	2.47	0.45
1:B:408:LEU:HB3	1:B:413:LEU:HG	1.98	0.45
1:B:424:PHE:CE1	1:B:468:GLU:HG2	2.52	0.45
1:C:408:LEU:HB3	1:C:413:LEU:HG	1.99	0.45
1:D:458:ILE:HG22	1:D:458:ILE:O	2.17	0.45
1:C:208:ASN:HD22	1:C:242:PRO:HD2	1.78	0.45
1:D:132:VAL:O	1:D:133:GLU:HB2	2.17	0.45
1:C:211:TYR:CZ	1:C:244:PRO:HB3	2.52	0.44
1:D:319:ALA:HA	1:D:324:PHE:CG	2.52	0.44
1:C:273:VAL:CA	1:C:285:TYR:HA	2.47	0.44
1:C:456:GLU:O	1:C:459:GLN:N	2.51	0.44
1:D:280:THR:HG22	1:D:282:LYS:HG3	1.99	0.44
1:A:323:GLU:HG2	1:B:17:SER:HB2	1.99	0.44
1:B:116:GLN:N	1:B:117:PRO:CD	2.80	0.44
1:B:161:SER:C	1:B:163:THR:N	2.74	0.44
1:A:157:LYS:O	1:A:157:LYS:HD3	2.17	0.44
1:A:181:ILE:HB	1:A:183:TYR:CE1	2.52	0.44
1:A:181:ILE:HG13	1:A:205:TYR:CZ	2.52	0.44
1:C:278:PRO:O	1:C:279:LYS:HD3	2.18	0.44
1:C:354:SER:HB2	1:C:359:ILE:HG22	1.98	0.44
1:D:120:GLY:HA3	2:D:503:PLG:C5A	2.47	0.44
1:A:137:ARG:HA	1:A:168:GLU:O	2.18	0.44
1:A:208:ASN:HD22	1:A:242:PRO:HD2	1.79	0.44
1:B:11:ASP:C	1:B:13:THR:N	2.75	0.44
1:C:435:ILE:HD12	1:C:448:PHE:CE1	2.53	0.44
1:A:387:ASN:ND2	3:A:600:THF:N1	2.63	0.44
1:B:145:ASP:OD2	1:B:174:VAL:HG22	2.17	0.44
1:B:181:ILE:HG13	1:B:205:TYR:CZ	2.53	0.44
1:C:270:ARG:NH1	1:C:274:ARG:HD3	2.32	0.44
1:C:465:LEU:O	1:C:469:VAL:HG23	2.18	0.44
1:D:417:ASP:O	1:D:421:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:TYR:CE1	1:B:207:ARG:HG3	2.52	0.44
1:B:208:ASN:HD22	1:B:242:PRO:HD2	1.80	0.44
1:B:444:THR:OG1	1:B:447:GLU:HG3	2.18	0.44
1:C:68:SER:HB3	1:D:484:PHE:OXT	2.18	0.44
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.31	0.44
1:A:235:LEU:HD23	1:A:328:GLN:CG	2.46	0.44
1:B:235:LEU:CD2	1:B:328:GLN:HG3	2.47	0.44
1:C:299:GLY:O	1:D:162:ALA:HB2	2.18	0.44
1:D:10:ARG:CB	1:D:10:ARG:NH2	2.81	0.44
1:D:280:THR:HG21	1:D:282:LYS:HD2	2.00	0.44
1:A:77:TYR:C	1:A:79:GLY:H	2.25	0.44
1:A:481:LEU:O	1:A:483:ASP:N	2.48	0.44
1:C:116:GLN:N	1:C:117:PRO:CD	2.80	0.44
1:C:183:TYR:CE2	1:C:210:ASP:HB3	2.52	0.44
1:C:273:VAL:HA	1:C:285:TYR:HA	2.00	0.44
1:C:364:ARG:NH2	1:C:392:ASP:OD2	2.50	0.44
1:A:279:LYS:C	1:A:281:GLY:H	2.26	0.43
1:B:350:VAL:HG21	1:B:360:LEU:HD23	1.99	0.43
1:B:455:ASP:O	1:B:456:GLU:HG2	2.18	0.43
1:C:92:LEU:HD11	1:C:310:ALA:HA	2.00	0.43
1:C:154:MSE:HE3	1:C:169:SER:OG	2.18	0.43
1:C:158:LYS:HE2	1:C:158:LYS:HB3	1.91	0.43
1:C:360:LEU:HD21	1:C:389:CYS:HB3	1.99	0.43
1:A:78:PRO:HG2	1:A:93:GLU:HG2	2.00	0.43
1:A:459:GLN:HA	1:A:462:VAL:CG1	2.43	0.43
1:B:372:ARG:NH1	1:B:397:ARG:NH1	2.59	0.43
1:B:413:LEU:H	1:B:413:LEU:CD2	2.30	0.43
1:D:152:GLY:HA2	1:D:163:THR:HB	1.99	0.43
1:A:299:GLY:O	1:B:162:ALA:HB2	2.18	0.43
1:A:417:ASP:O	1:A:421:VAL:HG23	2.19	0.43
1:C:121:SER:N	1:C:122:PRO:CD	2.82	0.43
1:D:144:PRO:HA	1:D:388:THR:CG2	2.48	0.43
1:D:145:ASP:OD2	1:D:174:VAL:HG22	2.19	0.43
1:D:413:LEU:H	1:D:413:LEU:CD2	2.31	0.43
1:D:450:GLU:O	1:D:454:GLY:CA	2.65	0.43
1:D:452:LEU:C	1:D:454:GLY:N	2.76	0.43
1:A:52:ALA:HA	1:A:404:GLY:HA3	2.00	0.43
1:B:121:SER:N	1:B:122:PRO:CD	2.82	0.43
1:B:361:MSE:HE2	1:B:403:LEU:CD1	2.43	0.43
1:B:372:ARG:HG3	1:B:372:ARG:HH11	1.82	0.43
1:C:66:GLY:O	1:D:481:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:GLY:HA3	2:C:502:PLG:C5A	2.48	0.43
1:C:319:ALA:HA	1:C:324:PHE:CD2	2.53	0.43
1:C:392:ASP:HB2	1:C:394:SER:CB	2.49	0.43
1:B:232:ILE:O	1:B:236:VAL:HG23	2.18	0.43
1:B:450:GLU:O	1:B:453:ALA:N	2.50	0.43
1:C:357:HIS:HD1	1:C:357:HIS:H	1.65	0.43
1:C:431:LEU:HD23	1:C:431:LEU:C	2.44	0.43
1:B:274:ARG:O	1:B:275:SER:CB	2.66	0.43
1:B:447:GLU:HA	1:B:450:GLU:HG2	2.01	0.43
1:C:134:PRO:HG3	1:D:166:PHE:CE1	2.53	0.43
1:C:162:ALA:HA	1:C:165:ILE:HD12	2.01	0.43
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.90	0.43
1:B:43:ARG:NH1	1:B:43:ARG:HG2	2.34	0.43
1:B:364:ARG:C	1:B:366:LYS:H	2.27	0.43
1:B:161:SER:O	1:B:162:ALA:C	2.62	0.43
1:C:52:ALA:HA	1:C:404:GLY:HA3	2.01	0.43
1:C:113:VAL:HG12	1:C:114:ASN:H	1.83	0.43
1:C:455:ASP:O	1:C:456:GLU:C	2.61	0.43
1:A:280:THR:O	1:A:282:LYS:N	2.52	0.43
1:B:257:LYS:NZ	2:B:501:PLG:C4A	2.82	0.43
1:D:10:ARG:O	1:D:12:ALA:N	2.52	0.43
1:D:445:LEU:HD12	1:D:445:LEU:C	2.44	0.43
1:A:439:MSE:O	1:A:440:ALA:C	2.61	0.42
1:A:462:VAL:HG13	1:A:463:ALA:H	1.85	0.42
1:B:159:LYS:HD3	1:B:165:ILE:HA	2.01	0.42
1:D:76:GLY:HA3	1:D:81:ARG:HA	2.01	0.42
1:D:142:ASP:HB3	1:D:145:ASP:HB2	2.00	0.42
1:A:107:ASP:C	1:A:109:GLN:H	2.26	0.42
1:A:183:TYR:CE2	1:A:210:ASP:HB3	2.54	0.42
1:C:14:LEU:C	1:C:16:ALA:N	2.77	0.42
1:C:435:ILE:CG1	1:C:458:ILE:HD13	2.49	0.42
1:D:319:ALA:HA	1:D:324:PHE:CD2	2.54	0.42
1:B:297:PHE:CD1	1:B:298:PRO:HA	2.54	0.42
1:C:154:MSE:O	1:C:154:MSE:HG3	2.18	0.42
1:D:334:ASN:HB3	1:D:418:PHE:CE2	2.55	0.42
1:A:156:ASP:HA	1:C:194:HIS:CD2	2.53	0.42
1:A:342:LEU:HD12	1:A:342:LEU:HA	1.88	0.42
1:B:139:MSE:HE3	1:B:170:MSE:CE	2.49	0.42
1:B:213:ARG:HH11	1:B:213:ARG:CG	2.32	0.42
1:C:14:LEU:CD2	1:D:322:THR:HG22	2.50	0.42
1:C:327:TYR:HB2	1:D:18:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:THR:O	1:C:443:ALA:N	2.51	0.42
1:D:143:LEU:N	1:D:144:PRO:HD2	2.34	0.42
1:A:170:MSE:HE1	1:A:189:ASN:HB3	2.02	0.42
1:A:319:ALA:HA	1:A:324:PHE:CG	2.54	0.42
1:A:323:GLU:O	1:A:326:ILE:HG23	2.20	0.42
1:A:354:SER:HB2	1:A:359:ILE:HG22	2.01	0.42
1:D:334:ASN:HB3	1:D:418:PHE:CD2	2.55	0.42
1:A:364:ARG:C	1:A:366:LYS:H	2.26	0.42
1:B:9:ASP:O	1:B:10:ARG:C	2.63	0.42
1:B:417:ASP:O	1:B:421:VAL:HG23	2.20	0.42
1:C:88:PHE:CE1	1:D:39:LYS:HB3	2.54	0.42
1:C:139:MSE:HE3	1:C:170:MSE:CE	2.49	0.42
1:C:342:LEU:HD12	1:C:342:LEU:HA	1.88	0.42
1:D:354:SER:HB2	1:D:359:ILE:HG22	2.01	0.42
1:D:451:LYS:HA	1:D:455:ASP:OD2	2.20	0.42
1:A:80:GLN:O	1:A:80:GLN:HG3	2.19	0.42
1:C:254:THR:CG2	2:C:502:PLG:H5A2	2.49	0.42
1:A:107:ASP:HA	1:A:108:PRO:HD2	1.91	0.42
1:B:75:GLU:HB2	1:B:83:TYR:HE2	1.84	0.42
1:C:278:PRO:CD	1:C:282:LYS:HE3	2.50	0.42
1:C:449:LYS:HB2	1:C:449:LYS:HZ3	1.84	0.42
1:D:450:GLU:C	1:D:452:LEU:H	2.28	0.42
1:A:481:LEU:HB3	1:A:482:PRO:HD2	2.02	0.42
1:B:215:ARG:HH11	1:B:219:ASP:CG	2.26	0.42
1:C:154:MSE:CE	1:C:169:SER:OG	2.68	0.42
1:D:10:ARG:HB3	1:D:10:ARG:NH2	2.35	0.42
1:D:139:MSE:HE3	1:D:170:MSE:CE	2.50	0.42
1:A:459:GLN:CA	1:A:462:VAL:HG12	2.45	0.41
1:B:107:ASP:OD2	1:B:109:GLN:HB2	2.19	0.41
1:B:384:CYS:SG	1:B:401:LEU:HD22	2.60	0.41
1:B:384:CYS:HB3	1:B:385:ASN:H	1.55	0.41
1:C:39:LYS:HB3	1:D:88:PHE:CE1	2.55	0.41
1:C:181:ILE:HB	1:C:183:TYR:CE1	2.55	0.41
1:C:451:LYS:O	1:C:452:LEU:C	2.62	0.41
1:D:183:TYR:CE2	1:D:210:ASP:HB3	2.55	0.41
1:A:137:ARG:NH2	1:C:154:MSE:HE1	2.35	0.41
1:A:323:GLU:HG2	1:B:17:SER:CB	2.50	0.41
1:A:372:ARG:HG3	1:A:372:ARG:HH11	1.84	0.41
1:A:462:VAL:CG1	1:A:463:ALA:N	2.84	0.41
1:B:14:LEU:C	1:B:16:ALA:N	2.76	0.41
1:B:148:HIS:CE1	1:B:150:THR:HG23	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LEU:HD23	1:A:197:LEU:C	2.44	0.41
1:A:319:ALA:HA	1:A:324:PHE:CD2	2.55	0.41
1:B:120:GLY:HA3	2:B:501:PLG:H5A2	2.03	0.41
1:C:59:ARG:HD3	1:D:23:SER:O	2.19	0.41
1:D:53:SER:O	1:D:257:LYS:HG2	2.21	0.41
1:D:448:PHE:O	1:D:452:LEU:HB2	2.20	0.41
1:B:137:ARG:HA	1:B:168:GLU:O	2.21	0.41
1:B:455:ASP:O	1:B:456:GLU:HB2	2.20	0.41
1:D:254:THR:HB	1:D:256:HIS:CE1	2.55	0.41
1:D:435:ILE:HD12	1:D:448:PHE:CE1	2.55	0.41
1:A:17:SER:CB	1:B:323:GLU:HG2	2.50	0.41
1:A:297:PHE:CD1	1:A:298:PRO:HA	2.55	0.41
1:A:83:TYR:OH	2:B:501:PLG:O	2.36	0.41
1:A:181:ILE:HD12	1:A:209:LEU:CD2	2.49	0.41
1:A:482:PRO:O	1:A:483:ASP:HB3	2.21	0.41
1:C:137:ARG:HA	1:C:168:GLU:O	2.21	0.41
1:D:52:ALA:HA	1:D:404:GLY:HA3	2.02	0.41
1:D:173:LYS:HE3	1:D:173:LYS:HB3	1.97	0.41
1:A:121:SER:N	1:A:122:PRO:CD	2.84	0.41
1:A:413:LEU:CD2	1:A:413:LEU:H	2.34	0.41
1:B:254:THR:OG1	1:B:257:LYS:HD2	2.21	0.41
1:B:273:VAL:HG13	1:B:284:THR:O	2.20	0.41
1:B:354:SER:HB2	1:B:359:ILE:HG22	2.02	0.41
1:B:388:THR:HA	1:B:398:PRO:HB3	2.03	0.41
1:C:323:GLU:HG3	1:D:14:LEU:HD13	2.02	0.41
1:D:140:GLY:O	1:D:171:PRO:HA	2.21	0.41
1:D:155:THR:HG22	1:D:158:LYS:H	1.86	0.41
1:D:397:ARG:N	1:D:398:PRO:CD	2.83	0.41
1:A:46:VAL:O	1:A:46:VAL:HG23	2.21	0.41
1:A:148:HIS:O	1:A:149:LEU:C	2.63	0.41
1:B:83:TYR:CD2	1:B:83:TYR:N	2.89	0.41
1:C:45:ARG:HG3	1:C:478:LEU:CD2	2.51	0.41
1:C:235:LEU:CD2	1:C:328:GLN:HE21	2.33	0.41
1:C:323:GLU:HB3	1:D:18:HIS:HB2	2.02	0.41
1:A:132:VAL:O	1:A:133:GLU:HB2	2.19	0.41
1:A:148:HIS:CE1	1:A:150:THR:HG23	2.55	0.41
1:A:361:MSE:O	1:A:400:GLY:CA	2.69	0.41
1:B:13:THR:HG23	1:B:14:LEU:N	2.36	0.41
1:B:107:ASP:C	1:B:109:GLN:H	2.29	0.41
1:B:215:ARG:CG	1:B:247:HIS:HB3	2.51	0.41
1:B:361:MSE:HE3	1:B:401:LEU:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG23	1:C:46:VAL:O	2.19	0.41
1:C:277:ASP:HB3	1:C:278:PRO:CD	2.42	0.41
1:C:361:MSE:HE2	1:C:403:LEU:CD1	2.38	0.41
1:D:235:LEU:CD2	1:D:328:GLN:HG3	2.49	0.41
1:D:408:LEU:HB3	1:D:413:LEU:HG	2.03	0.41
1:D:434:GLN:C	1:D:436:GLN:N	2.77	0.41
1:A:32:GLU:O	1:A:36:ILE:HG13	2.21	0.41
1:A:82:TYR:CE1	1:A:297:PHE:HE2	2.39	0.41
1:A:88:PHE:CE1	1:B:39:LYS:HB3	2.56	0.41
1:B:319:ALA:HA	1:B:324:PHE:CG	2.56	0.41
1:B:452:LEU:HD13	1:B:452:LEU:C	2.46	0.41
1:C:227:ALA:HB2	1:C:248:CYS:SG	2.61	0.41
1:C:227:ALA:HB3	1:C:251:VAL:HG22	2.02	0.41
1:C:364:ARG:C	1:C:366:LYS:H	2.29	0.41
1:A:40:GLU:HG3	1:A:44:GLN:HE21	1.85	0.40
1:B:372:ARG:HH12	1:B:397:ARG:HH12	1.67	0.40
1:B:457:LYS:O	1:B:460:SER:HB2	2.21	0.40
1:C:78:PRO:HG2	1:C:93:GLU:HG2	2.03	0.40
1:A:141:LEU:O	1:A:142:ASP:C	2.64	0.40
1:B:431:LEU:C	1:B:431:LEU:CD2	2.93	0.40
1:C:153:PHE:CD2	1:C:160:ILE:HB	2.56	0.40
1:D:107:ASP:C	1:D:109:GLN:H	2.29	0.40
1:D:439:MSE:O	1:D:441:THR:N	2.54	0.40
1:D:473:ALA:O	1:D:475:ASN:N	2.55	0.40
1:A:408:LEU:HB3	1:A:413:LEU:HG	2.02	0.40
1:C:364:ARG:HH21	1:C:392:ASP:CG	2.29	0.40
1:C:449:LYS:NZ	1:C:449:LYS:CB	2.83	0.40
1:C:356:ASN:HB2	1:C:357:HIS:H	1.66	0.40
1:D:132:VAL:HG12	1:D:136:GLY:HA3	2.04	0.40
1:D:235:LEU:CD2	1:D:328:GLN:HE21	2.35	0.40
1:D:259:LEU:HD12	1:D:259:LEU:HA	1.88	0.40
1:A:92:LEU:HD11	1:A:310:ALA:HA	2.03	0.40
1:A:277:ASP:CB	1:A:282:LYS:H	2.32	0.40
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.89	0.40
1:A:319:ALA:O	1:A:324:PHE:CD2	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/478 (100%)	401 (84%)	53 (11%)	22 (5%)	2	7
1	B	476/478 (100%)	408 (86%)	53 (11%)	15 (3%)	3	13
1	C	476/478 (100%)	397 (83%)	52 (11%)	27 (6%)	1	4
1	D	476/478 (100%)	405 (85%)	54 (11%)	17 (4%)	2	11
All	All	1904/1912 (100%)	1611 (85%)	212 (11%)	81 (4%)	2	8

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	VAL
1	A	278	PRO
1	A	281	GLY
1	A	393	LYS
1	B	10	ARG
1	B	385	ASN
1	C	12	ALA
1	C	276	VAL
1	C	278	PRO
1	C	385	ASN
1	C	394	SER
1	C	398	PRO
1	C	438	HIS
1	C	440	ALA
1	C	443	ALA
1	C	456	GLU
1	D	440	ALA
1	D	452	LEU
1	A	9	ASP
1	A	10	ARG
1	A	11	ASP
1	A	12	ALA

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Mol	Chain	Res	Type
1	A	398	PRO
1	A	454	GLY
1	A	456	GLU
1	A	474	SER
1	B	395	ALA
1	B	398	PRO
1	B	453	ALA
1	C	75	GLU
1	C	282	LYS
1	C	283	GLU
1	C	455	ASP
1	C	474	SER
1	D	11	ASP
1	D	258	THR
1	D	394	SER
1	D	451	LYS
1	D	474	SER
1	A	75	GLU
1	A	438	HIS
1	A	440	ALA
1	B	15	TRP
1	B	75	GLU
1	B	454	GLY
1	B	456	GLU
1	B	474	SER
1	C	275	SER
1	C	277	ASP
1	C	285	TYR
1	C	399	SER
1	D	75	GLU
1	A	399	SER
1	A	450	GLU
1	B	258	THR
1	B	275	SER
1	B	278	PRO
1	B	438	HIS
1	B	482	PRO
1	C	273	VAL
1	C	281	GLY
1	C	441	THR
1	C	444	THR
1	D	8	ALA

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Mol	Chain	Res	Type
1	D	13	THR
1	D	456	GLU
1	A	103	ALA
1	A	257	LYS
1	A	451	LYS
1	C	103	ALA
1	C	413	LEU
1	D	273	VAL
1	D	275	SER
1	D	413	LEU
1	D	454	GLY
1	D	457	LYS
1	D	482	PRO
1	A	150	THR
1	A	413	LEU
1	C	272	GLY
1	C	482	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	394/383 (103%)	382 (97%)	12 (3%)	36	70
1	B	394/383 (103%)	373 (95%)	21 (5%)	20	52
1	C	394/383 (103%)	371 (94%)	23 (6%)	18	49
1	D	394/383 (103%)	373 (95%)	21 (5%)	20	52
All	All	1576/1532 (103%)	1499 (95%)	77 (5%)	22	54

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	MET
1	A	73	TYR
1	A	87	GLU
1	A	113	VAL

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Mol	Chain	Res	Type
1	A	171	PRO
1	A	188	GLU
1	A	342	LEU
1	A	413	LEU
1	A	435	ILE
1	A	445	LEU
1	A	450	GLU
1	A	452	LEU
1	B	73	TYR
1	B	87	GLU
1	B	113	VAL
1	B	157	LYS
1	B	171	PRO
1	B	188	GLU
1	B	275	SER
1	B	277	ASP
1	B	298	PRO
1	B	342	LEU
1	B	384	CYS
1	B	385	ASN
1	B	387	ASN
1	B	388	THR
1	B	392	ASP
1	B	393	LYS
1	B	413	LEU
1	B	435	ILE
1	B	449	LYS
1	B	456	GLU
1	B	483	ASP
1	C	73	TYR
1	C	75	GLU
1	C	87	GLU
1	C	113	VAL
1	C	156	ASP
1	C	161	SER
1	C	171	PRO
1	C	188	GLU
1	C	231	HIS
1	C	273	VAL
1	C	274	ARG
1	C	342	LEU
1	C	385	ASN

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Mol	Chain	Res	Type
1	C	387	ASN
1	C	392	ASP
1	C	398	PRO
1	C	413	LEU
1	C	435	ILE
1	C	438	HIS
1	C	444	THR
1	C	449	LYS
1	C	450	GLU
1	C	484	PHE
1	D	73	TYR
1	D	87	GLU
1	D	113	VAL
1	D	145	ASP
1	D	155	THR
1	D	171	PRO
1	D	188	GLU
1	D	231	HIS
1	D	278	PRO
1	D	342	LEU
1	D	389	CYS
1	D	397	ARG
1	D	402	ARG
1	D	413	LEU
1	D	435	ILE
1	D	444	THR
1	D	447	GLU
1	D	452	LEU
1	D	456	GLU
1	D	457	LYS
1	D	482	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	70	ASN
1	A	71	ASN
1	A	102	GLN
1	A	194	HIS
1	A	231	HIS
1	A	247	HIS

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Mol	Chain	Res	Type
1	A	328	GLN
1	A	423	HIS
1	A	471	ASN
1	B	70	ASN
1	B	71	ASN
1	B	102	GLN
1	B	208	ASN
1	B	231	HIS
1	B	247	HIS
1	B	328	GLN
1	B	385	ASN
1	B	387	ASN
1	B	423	HIS
1	B	471	ASN
1	B	475	ASN
1	C	44	GLN
1	C	70	ASN
1	C	71	ASN
1	C	102	GLN
1	C	194	HIS
1	C	231	HIS
1	C	247	HIS
1	C	328	GLN
1	C	385	ASN
1	C	387	ASN
1	C	423	HIS
1	C	471	ASN
1	C	475	ASN
1	D	70	ASN
1	D	71	ASN
1	D	102	GLN
1	D	194	HIS
1	D	231	HIS
1	D	247	HIS
1	D	318	GLN
1	D	328	GLN
1	D	387	ASN
1	D	423	HIS
1	D	438	HIS
1	D	471	ASN
1	D	475	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLG	B	501	-	20,20,20	5.06	12 (60%)	26,28,28	3.41	13 (50%)
2	PLG	C	502	1	20,20,20	4.29	12 (60%)	26,28,28	2.87	9 (34%)
3	THF	B	601	-	32,36,36	3.24	17 (53%)	37,50,50	2.84	12 (32%)
2	PLG	D	503	1	20,20,20	4.49	13 (65%)	26,28,28	2.84	9 (34%)
3	THF	D	602	-	32,36,36	3.32	19 (59%)	37,50,50	3.27	13 (35%)
3	THF	A	600	-	32,36,36	3.25	14 (43%)	37,50,50	3.05	16 (43%)
2	PLG	A	500	-	20,20,20	4.99	14 (70%)	26,28,28	3.42	12 (46%)

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	PLG	B	501	-	-	4/12/12/12	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLG	C	502	1	-	5/12/12/12	0/1/1/1
3	THF	B	601	-	-	8/22/37/37	0/3/3/3
2	PLG	D	503	1	-	3/12/12/12	0/1/1/1
3	THF	D	602	-	-	7/22/37/37	0/3/3/3
3	THF	A	600	-	-	4/22/37/37	0/3/3/3
2	PLG	A	500	-	-	4/12/12/12	0/1/1/1

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLG	C4A-C4	-11.84	1.34	1.52
2	B	501	PLG	C3-C4	11.71	1.57	1.40
2	D	503	PLG	C3-C4	11.64	1.57	1.40
2	A	500	PLG	C3-C4	11.49	1.56	1.40
2	A	500	PLG	C4A-C4	-11.45	1.35	1.52
2	C	502	PLG	C3-C4	10.56	1.55	1.40
2	C	502	PLG	C3-C2	9.81	1.51	1.41
3	A	600	THF	O4-C4	9.60	1.41	1.23
3	B	601	THF	O4-C4	9.20	1.40	1.23
3	D	602	THF	O4-C4	8.65	1.39	1.23
2	D	503	PLG	C3-C2	8.63	1.49	1.41
2	B	501	PLG	C3-C2	8.47	1.49	1.41
3	D	602	THF	C7-N8	7.49	1.37	1.28
2	A	500	PLG	C3-C2	7.37	1.48	1.41
2	D	503	PLG	C5-C4	7.07	1.50	1.40
2	A	500	PLG	C5-C4	6.69	1.49	1.40
3	A	600	THF	C7-N8	6.68	1.36	1.28
3	B	601	THF	C7-N8	6.48	1.36	1.28
2	C	502	PLG	C5-C4	5.97	1.48	1.40
3	A	600	THF	C2-NA2	5.97	1.48	1.34
3	D	602	THF	C2-NA2	5.84	1.47	1.34
3	B	601	THF	C2-NA2	5.81	1.47	1.34
2	B	501	PLG	C5-C4	5.77	1.48	1.40
2	B	501	PLG	P-OP4	-5.53	1.42	1.60
2	A	500	PLG	P-OP4	-5.49	1.43	1.60
2	C	502	PLG	P-OP4	-5.28	1.43	1.60
3	D	602	THF	C8A-N8	5.03	1.41	1.36
3	A	600	THF	C2-N3	-4.90	1.21	1.33
3	B	601	THF	C2-N3	-4.90	1.21	1.33
2	D	503	PLG	P-OP4	-4.88	1.44	1.60
2	D	503	PLG	CA-C	4.76	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	PLG	CA-C	4.75	1.62	1.50
3	D	602	THF	CP1-N5	4.65	1.51	1.45
3	D	602	THF	C2-N3	-4.62	1.21	1.33
2	C	502	PLG	CA-C	4.60	1.62	1.50
2	D	503	PLG	C6-C5	4.49	1.46	1.37
2	B	501	PLG	CA-C	4.41	1.61	1.50
3	B	601	THF	CP1-N5	4.38	1.51	1.45
2	B	501	PLG	C6-C5	4.28	1.46	1.37
3	D	602	THF	C12-C11	4.22	1.45	1.39
2	D	503	PLG	C2-N1	4.19	1.41	1.33
2	A	500	PLG	C6-C5	4.14	1.45	1.37
2	B	501	PLG	P-OP3	-4.05	1.39	1.54
2	B	501	PLG	C2-N1	4.04	1.41	1.33
2	C	502	PLG	P-OP3	-4.02	1.39	1.54
2	A	500	PLG	P-OP3	-4.01	1.39	1.54
2	D	503	PLG	P-OP3	-3.99	1.40	1.54
2	C	502	PLG	C6-C5	3.97	1.45	1.37
3	A	600	THF	CP1-N5	3.94	1.50	1.45
3	A	600	THF	C8A-N8	3.90	1.40	1.36
2	A	500	PLG	C2-N1	3.81	1.40	1.33
3	A	600	THF	C16-C11	3.74	1.45	1.39
3	B	601	THF	C12-C11	3.72	1.45	1.39
3	B	601	THF	C16-C11	3.70	1.45	1.39
3	B	601	THF	C8A-N8	3.65	1.40	1.36
3	D	602	THF	CA-CT	3.51	1.61	1.52
3	B	601	THF	C16-C15	3.48	1.44	1.38
3	A	600	THF	C16-C15	3.43	1.44	1.38
2	D	503	PLG	C4A-C4	3.43	1.57	1.52
3	B	601	THF	C15-C14	3.43	1.45	1.39
2	C	502	PLG	C2-N1	3.42	1.39	1.33
3	D	602	THF	C16-C11	3.36	1.44	1.39
2	A	500	PLG	P-OP2	-3.22	1.42	1.54
3	A	600	THF	C12-C11	3.20	1.44	1.39
3	B	601	THF	C14-N10	3.15	1.47	1.38
3	D	602	THF	C15-C14	3.15	1.44	1.39
3	A	600	THF	CA-CT	3.11	1.60	1.52
2	D	503	PLG	P-OP2	-3.06	1.43	1.54
3	A	600	THF	CG-CD	3.00	1.57	1.50
3	A	600	THF	C15-C14	2.95	1.44	1.39
3	D	602	THF	C16-C15	2.90	1.43	1.38
3	D	602	THF	C14-N10	2.87	1.46	1.38
2	B	501	PLG	P-OP2	-2.85	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PLG	CA-N	-2.78	1.39	1.46
2	C	502	PLG	P-OP2	-2.77	1.44	1.54
3	D	602	THF	C13-C12	2.69	1.43	1.38
3	A	600	THF	C14-N10	2.69	1.46	1.38
3	B	601	THF	C13-C12	2.68	1.43	1.38
2	D	503	PLG	C6-N1	2.67	1.39	1.34
2	C	502	PLG	C4A-C4	2.65	1.55	1.52
3	B	601	THF	CA-CT	2.61	1.59	1.52
3	A	600	THF	CB-CA	-2.58	1.47	1.53
2	D	503	PLG	CA-N	2.57	1.53	1.46
2	C	502	PLG	C6-N1	2.49	1.39	1.34
3	B	601	THF	CG-CD	2.48	1.56	1.50
2	A	500	PLG	OXT-C	-2.46	1.22	1.30
2	B	501	PLG	C6-N1	2.45	1.39	1.34
2	A	500	PLG	C6-N1	2.44	1.39	1.34
2	A	500	PLG	CA-N	-2.42	1.40	1.46
2	C	502	PLG	CA-N	2.39	1.52	1.46
3	B	601	THF	C13-C14	2.33	1.43	1.39
2	D	503	PLG	C5A-C5	2.27	1.56	1.50
3	D	602	THF	CB-CA	-2.26	1.48	1.53
3	D	602	THF	CG-CD	2.21	1.55	1.50
3	B	601	THF	CB-CA	-2.14	1.48	1.53
3	D	602	THF	CA-N	2.13	1.50	1.45
2	A	500	PLG	C5A-C5	2.10	1.56	1.50
3	D	602	THF	C13-C14	2.10	1.42	1.39
3	B	601	THF	C9-N10	2.07	1.49	1.45
3	D	602	THF	O3-CP1	2.05	1.46	1.40
3	D	602	THF	C9-N10	2.04	1.49	1.45

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	THF	C7-N8-C8A	13.39	127.43	115.47
3	A	600	THF	C7-N8-C8A	10.22	124.61	115.47
2	B	501	PLG	C4A-N-CA	9.91	124.25	112.72
3	B	601	THF	C7-N8-C8A	9.32	123.80	115.47
2	A	500	PLG	C4A-N-CA	9.16	123.39	112.72
2	A	500	PLG	OP3-P-OP4	8.73	129.43	106.67
3	A	600	THF	C8A-C4A-N5	-8.58	108.24	119.80
3	B	601	THF	C8A-C4A-N5	-8.47	108.38	119.80
2	C	502	PLG	OP3-P-OP4	8.47	128.74	106.67
2	B	501	PLG	OP3-P-OP4	8.30	128.32	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	503	PLG	OP4-C5A-C5	8.26	124.85	109.36
2	D	503	PLG	OP3-P-OP4	8.21	128.07	106.67
3	D	602	THF	C8A-C4A-N5	-8.20	108.75	119.80
2	C	502	PLG	OP4-C5A-C5	7.65	123.69	109.36
2	A	500	PLG	OP4-C5A-C5	6.76	122.02	109.36
2	B	501	PLG	OP4-C5A-C5	6.59	121.71	109.36
3	D	602	THF	N1-C2-N3	5.67	133.69	123.32
3	A	600	THF	N1-C2-N3	5.59	133.56	123.32
3	B	601	THF	N1-C2-N3	5.53	133.44	123.32
3	A	600	THF	NA2-C2-N3	-4.80	110.29	119.67
3	B	601	THF	NA2-C2-N3	-4.80	110.29	119.67
3	D	602	THF	NA2-C2-N3	-4.69	110.52	119.67
2	A	500	PLG	C4-C4A-N	4.39	119.61	111.50
2	A	500	PLG	C6-N1-C2	4.29	126.97	119.20
2	B	501	PLG	C6-N1-C2	4.17	126.77	119.20
2	D	503	PLG	C6-N1-C2	4.13	126.70	119.20
2	C	502	PLG	C6-N1-C2	4.05	126.55	119.20
2	C	502	PLG	O3-C3-C2	4.00	125.88	117.58
2	B	501	PLG	C4-C4A-N	3.75	118.43	111.50
3	A	600	THF	CT-CA-N	3.55	118.80	110.57
3	A	600	THF	C11-C-N	3.52	123.57	117.04
3	D	602	THF	CT-CA-N	3.45	118.58	110.57
2	D	503	PLG	O3-C3-C2	3.44	124.70	117.58
2	B	501	PLG	O3-C3-C2	3.40	124.63	117.58
2	A	500	PLG	O3-C3-C2	3.30	124.43	117.58
3	D	602	THF	C12-C13-C14	-3.11	116.72	120.30
3	A	600	THF	C13-C14-N10	-3.02	114.14	120.96
2	C	502	PLG	C5A-C5-C6	-2.90	114.64	119.36
3	B	601	THF	C12-C13-C14	-2.81	117.06	120.30
3	B	601	THF	C11-C-N	2.70	122.04	117.04
3	A	600	THF	C12-C13-C14	-2.69	117.20	120.30
2	A	500	PLG	C5A-C5-C6	-2.63	115.07	119.36
2	A	500	PLG	OXT-C-O	-2.62	116.59	123.33
2	C	502	PLG	C3-C2-N1	-2.62	117.66	120.96
3	B	601	THF	C13-C14-N10	-2.59	115.11	120.96
3	D	602	THF	C11-C-N	2.59	121.84	117.04
3	A	600	THF	C13-C12-C11	2.57	123.54	120.80
2	D	503	PLG	OXT-C-O	-2.56	116.74	123.33
2	D	503	PLG	C5A-C5-C6	-2.52	115.25	119.36
2	C	502	PLG	OXT-C-O	-2.51	116.88	123.33
2	B	501	PLG	OXT-C-O	-2.50	116.91	123.33
3	B	601	THF	CT-CA-N	2.50	116.36	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	PLG	C3-C2-N1	-2.48	117.83	120.96
2	B	501	PLG	OXT-C-CA	2.44	122.08	112.81
3	A	600	THF	O-C-N	-2.43	117.85	122.47
2	D	503	PLG	C3-C2-N1	-2.42	117.91	120.96
3	B	601	THF	CB-CG-CD	2.39	118.86	112.49
2	D	503	PLG	OXT-C-CA	2.38	121.87	112.81
2	A	500	PLG	OP3-P-OP1	-2.38	101.58	110.83
2	C	502	PLG	OXT-C-CA	2.36	121.78	112.81
2	A	500	PLG	C3-C2-N1	-2.36	117.98	120.96
3	A	600	THF	C9-N10-C14	2.34	127.95	122.00
3	D	602	THF	O2-CT-CA	2.30	121.28	113.51
3	D	602	THF	C13-C14-N10	-2.28	115.81	120.96
2	A	500	PLG	OXT-C-CA	2.26	121.42	112.81
3	A	600	THF	C15-C14-C13	2.25	122.03	119.04
3	D	602	THF	C13-C12-C11	2.24	123.19	120.80
3	D	602	THF	CB-CG-CD	2.23	118.44	112.49
3	D	602	THF	C15-C14-C13	2.22	121.99	119.04
3	B	601	THF	C13-C12-C11	2.21	123.16	120.80
3	D	602	THF	O3-CP1-N5	2.15	117.87	112.31
2	B	501	PLG	C4A-C4-C3	2.14	122.83	119.98
2	B	501	PLG	OP3-P-OP1	-2.14	102.51	110.83
2	C	502	PLG	OP3-P-OP1	-2.13	102.53	110.83
2	A	500	PLG	C5-C6-N1	-2.12	120.38	123.83
3	A	600	THF	O3-CP1-N5	2.12	117.80	112.31
2	D	503	PLG	OP3-P-OP1	-2.11	102.63	110.83
3	A	600	THF	O2-CT-CA	2.10	120.62	113.51
2	B	501	PLG	C5A-C5-C6	-2.10	115.94	119.36
2	B	501	PLG	C5-C6-N1	-2.07	120.46	123.83
3	A	600	THF	CB-CG-CD	2.07	118.01	112.49
3	B	601	THF	O3-CP1-N5	2.05	117.62	112.31
3	B	601	THF	C15-C14-C13	2.04	121.75	119.04
3	A	600	THF	OE2-CD-CG	2.03	120.41	114.00

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	PLG	C3-C4-C4A-N
2	A	500	PLG	C5-C4-C4A-N
2	A	500	PLG	C4-C5-C5A-OP4
2	A	500	PLG	C6-C5-C5A-OP4
2	B	501	PLG	C5-C4-C4A-N

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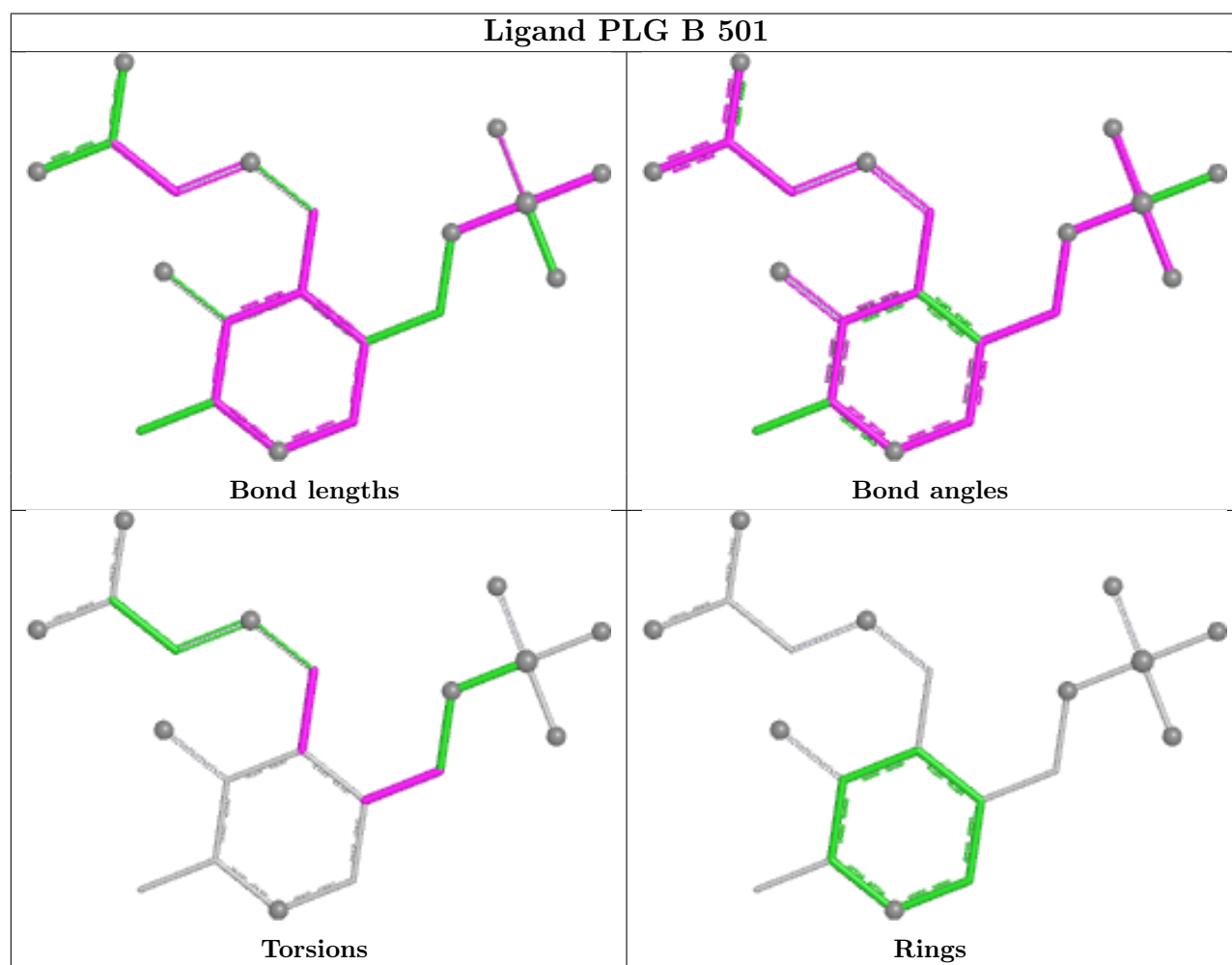
Mol	Chain	Res	Type	Atoms
2	B	501	PLG	C4-C5-C5A-OP4
2	B	501	PLG	C6-C5-C5A-OP4
2	C	502	PLG	C4-C5-C5A-OP4
2	C	502	PLG	C6-C5-C5A-OP4
2	D	503	PLG	C4-C5-C5A-OP4
2	D	503	PLG	C6-C5-C5A-OP4
3	A	600	THF	C11-C-N-CA
3	D	602	THF	N-CA-CB-CG
3	D	602	THF	O-C-N-CA
3	D	602	THF	C11-C-N-CA
3	D	602	THF	CT-CA-N-C
3	A	600	THF	O-C-N-CA
3	B	601	THF	O-C-C11-C12
3	B	601	THF	N-C-C11-C12
3	B	601	THF	N-C-C11-C16
3	B	601	THF	O-C-C11-C16
2	C	502	PLG	C4-C4A-N-CA
2	D	503	PLG	C4-C4A-N-CA
3	A	600	THF	CT-CA-CB-CG
3	D	602	THF	CB-CA-CT-O2
3	D	602	THF	CB-CA-CT-O1
3	D	602	THF	CT-CA-CB-CG
2	B	501	PLG	C3-C4-C4A-N
2	C	502	PLG	OXT-C-CA-N
2	C	502	PLG	O-C-CA-N
3	A	600	THF	CT-CA-N-C
3	B	601	THF	N-CA-CB-CG
3	B	601	THF	C6-C9-N10-C14
3	B	601	THF	OE1-CD-CG-CB
3	B	601	THF	OE2-CD-CG-CB

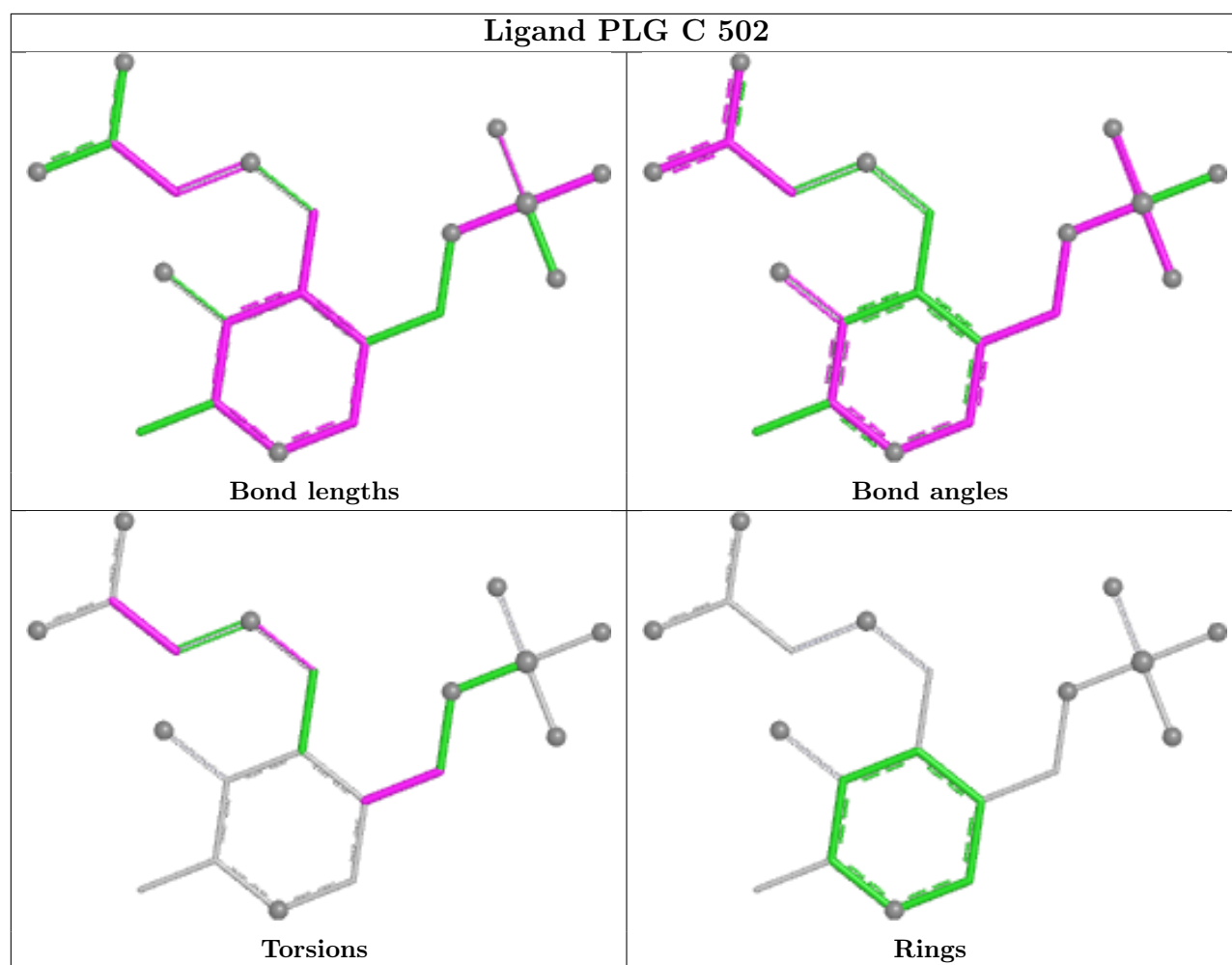
There are no ring outliers.

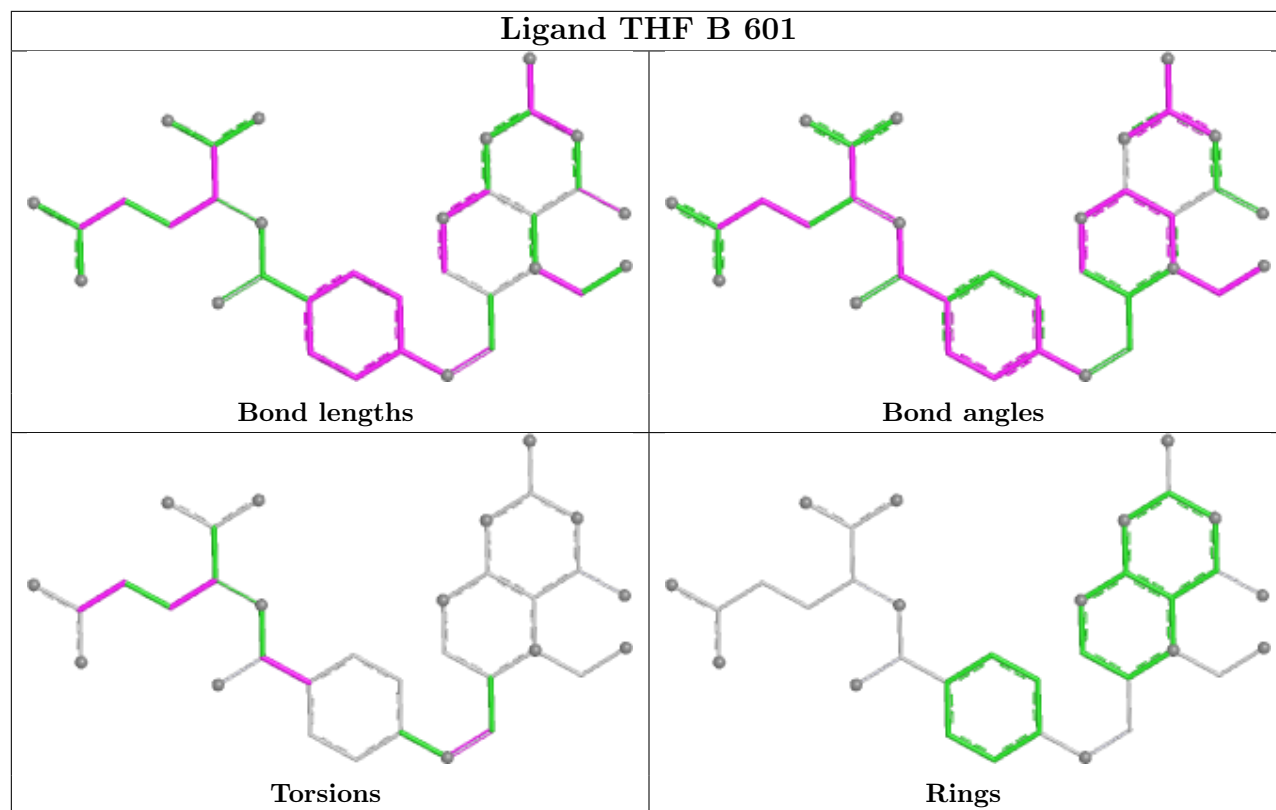
7 monomers are involved in 16 short contacts:

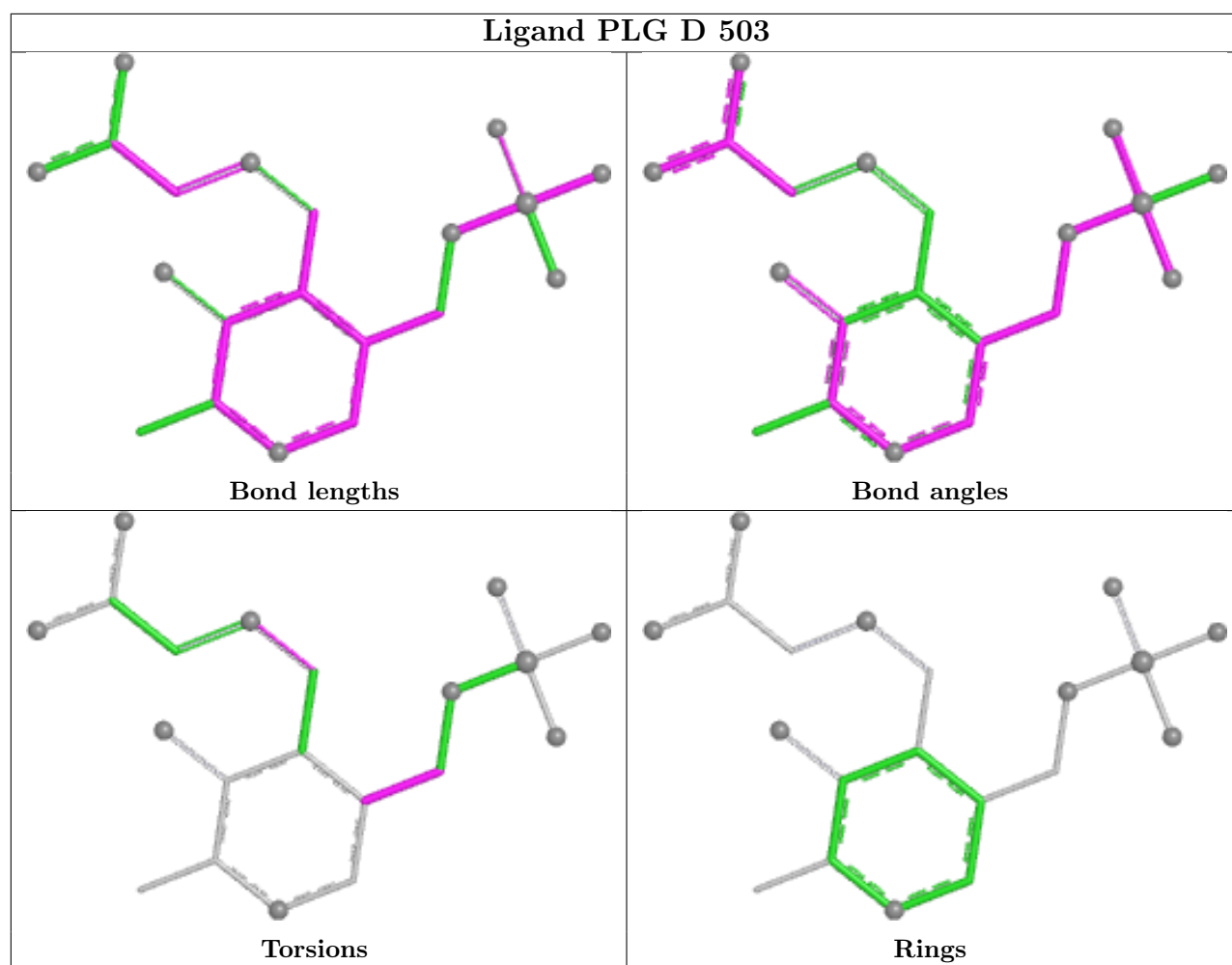
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PLG	5	0
2	C	502	PLG	3	0
3	B	601	THF	1	0
2	D	503	PLG	2	0
3	D	602	THF	1	0
3	A	600	THF	3	0
2	A	500	PLG	1	0

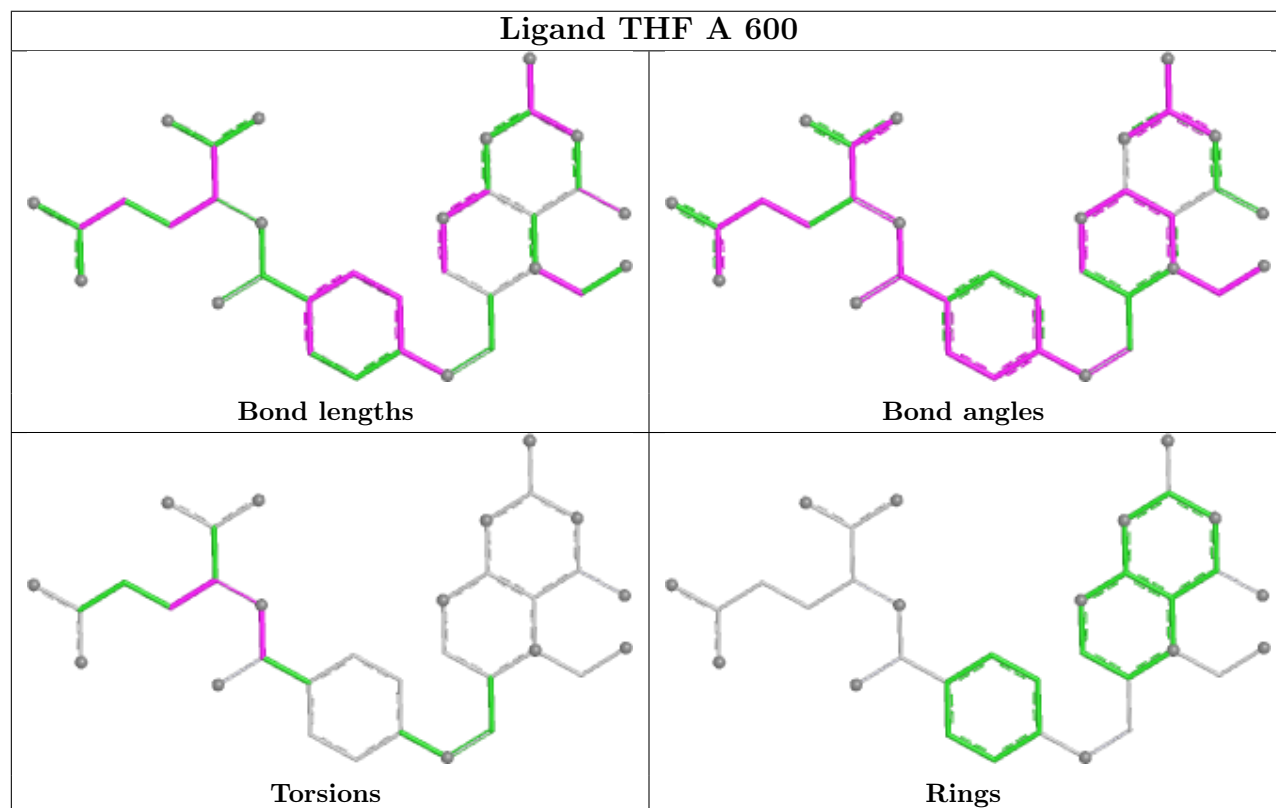
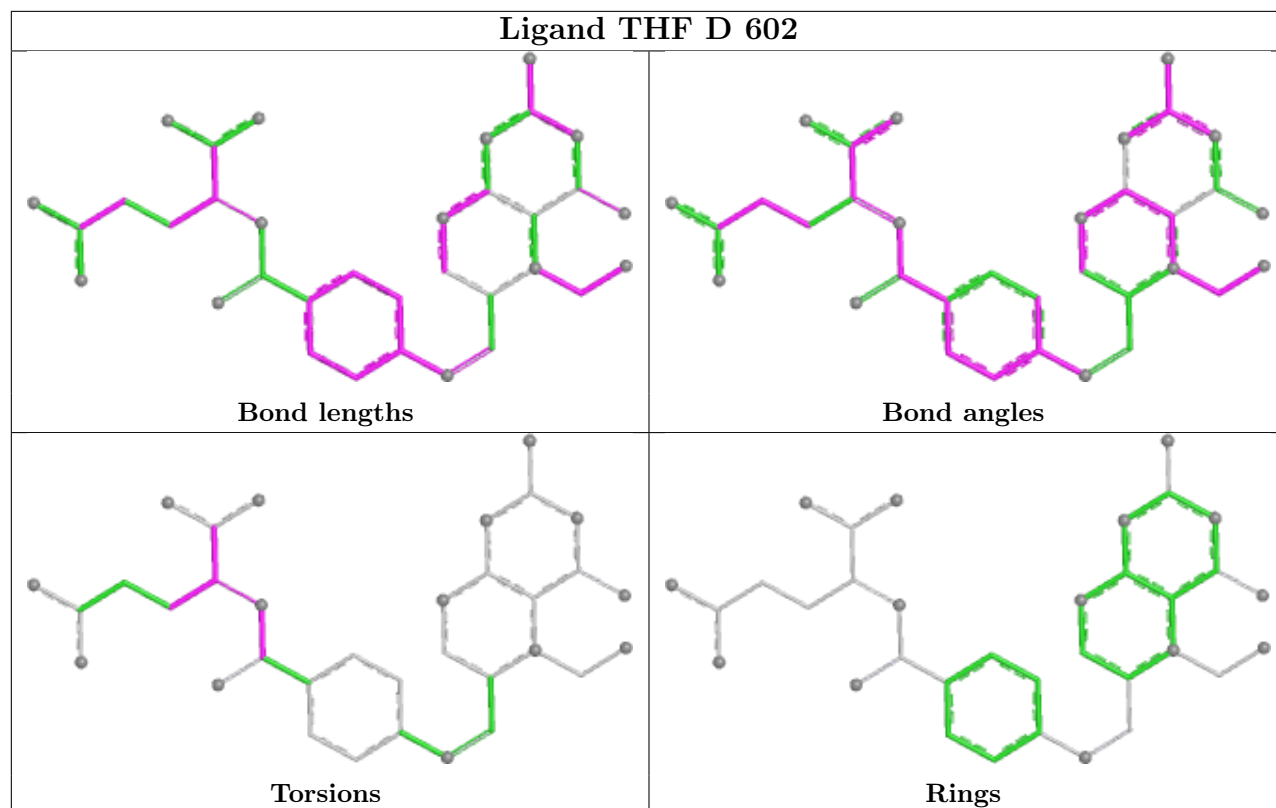
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

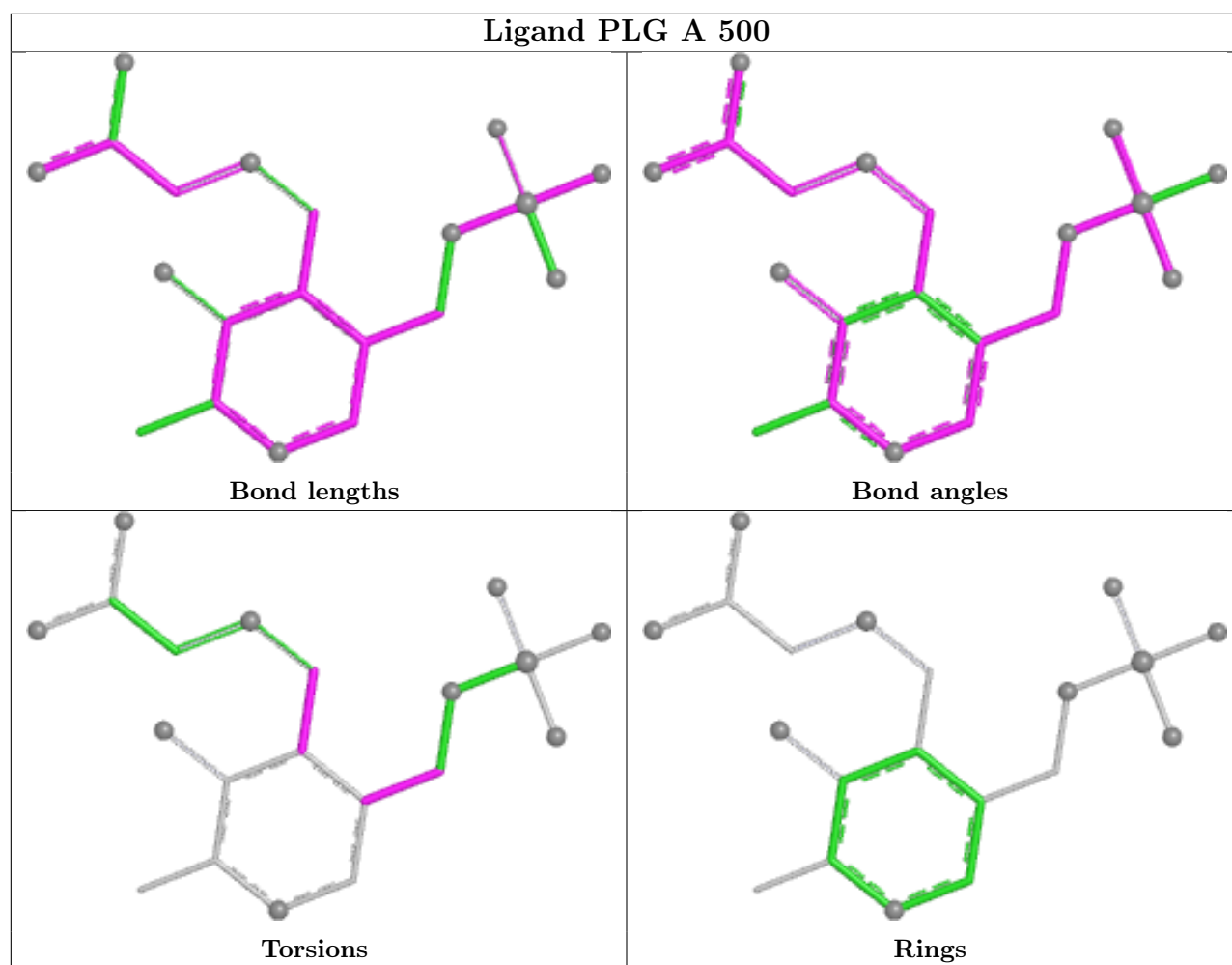












5.7 Other polymers [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	467/478 (97%)	0.33	19 (4%) 41 33	44, 79, 140, 151	0
1	B	467/478 (97%)	0.05	7 (1%) 72 64	42, 68, 139, 151	0
1	C	467/478 (97%)	0.29	14 (2%) 52 43	44, 79, 133, 151	0
1	D	467/478 (97%)	0.31	12 (2%) 57 48	44, 81, 138, 151	0
All	All	1868/1912 (97%)	0.24	52 (2%) 55 46	42, 76, 139, 151	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	362	ASP	4.8
1	D	484	PHE	4.5
1	A	368	THR	3.9
1	A	373	ALA	3.9
1	A	433	LEU	3.9
1	C	484	PHE	3.9
1	D	407	ALA	3.8
1	A	484	PHE	3.8
1	A	370	GLY	3.7
1	A	429	ILE	3.5
1	C	175	TYR	3.5
1	A	365	SER	3.3
1	A	364	ARG	3.3
1	D	371	GLY	3.1
1	B	484	PHE	3.1
1	D	452	LEU	3.1
1	C	15	TRP	3.0
1	A	273	VAL	3.0
1	C	367	GLY	3.0
1	A	444	THR	3.0
1	A	445	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	280	THR	2.9
1	D	339	SER	2.8
1	B	276	VAL	2.7
1	B	437	SER	2.7
1	A	347	TYR	2.6
1	B	14	LEU	2.6
1	C	435	ILE	2.6
1	D	363	LEU	2.6
1	B	278	PRO	2.4
1	B	365	SER	2.4
1	C	9	ASP	2.4
1	C	440	ALA	2.4
1	C	18	HIS	2.4
1	A	10	ARG	2.4
1	D	70	ASN	2.3
1	A	392	ASP	2.3
1	D	49	GLU	2.3
1	D	175	TYR	2.2
1	A	105	HIS	2.2
1	C	380	CYS	2.2
1	C	442	LYS	2.2
1	D	273	VAL	2.1
1	C	85	GLY	2.1
1	C	368	THR	2.1
1	A	7	MET	2.1
1	D	84	GLY	2.1
1	C	366	LYS	2.0
1	D	396	LEU	2.0
1	A	371	GLY	2.0
1	B	393	LYS	2.0
1	A	379	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

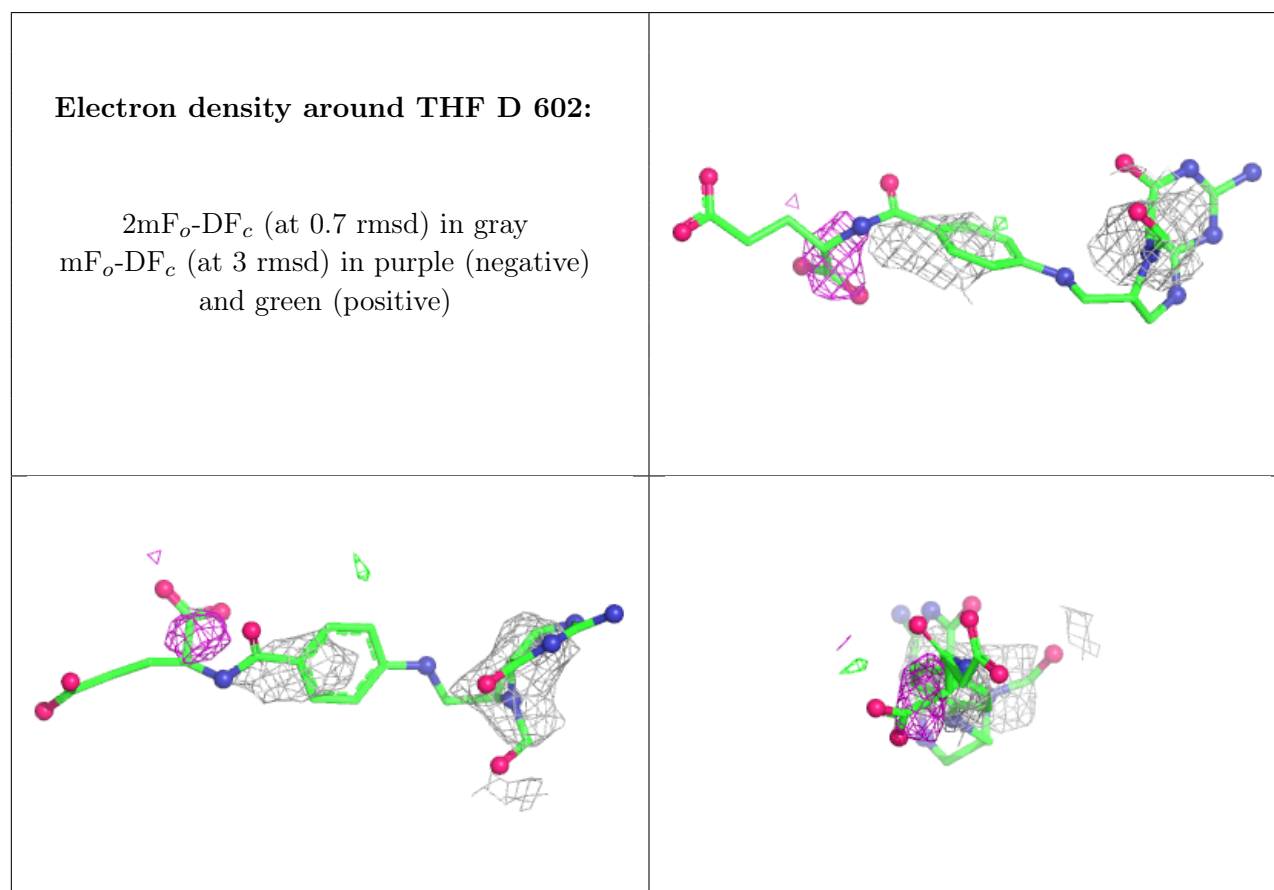
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

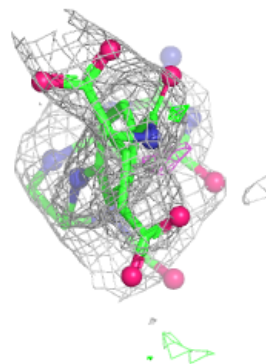
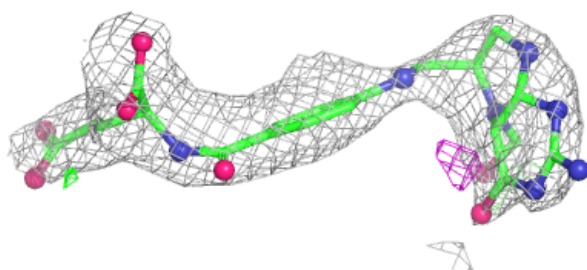
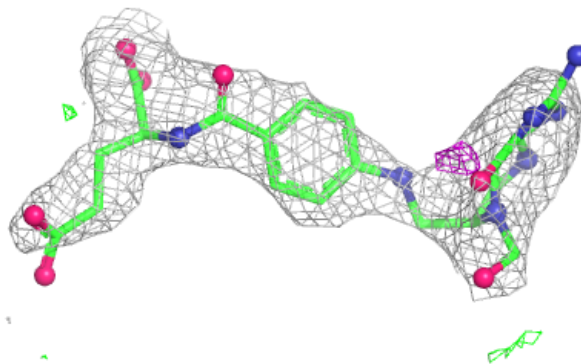
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	THF	D	602	34/34	0.80	0.19	151,151,151,151	0
3	THF	A	600	34/34	0.89	0.13	106,106,106,106	0
2	PLG	C	502	20/20	0.91	0.13	77,77,112,112	0
3	THF	B	601	34/34	0.92	0.14	132,132,132,132	0
2	PLG	D	503	20/20	0.93	0.11	88,88,118,118	0
2	PLG	B	501	20/20	0.95	0.10	79,79,88,88	0
2	PLG	A	500	20/20	0.96	0.08	70,70,91,91	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



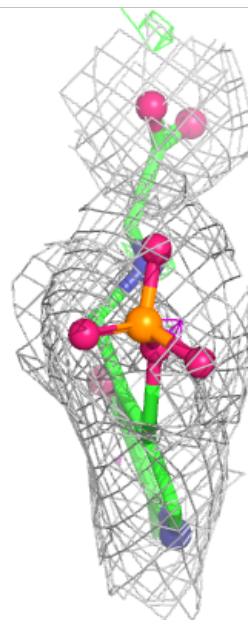
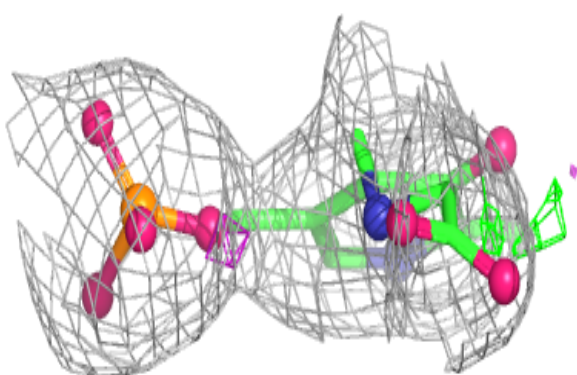
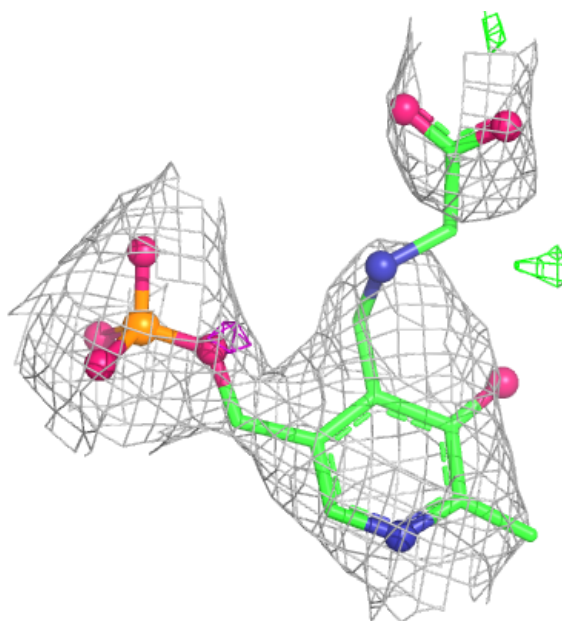
Electron density around THF A 600:

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



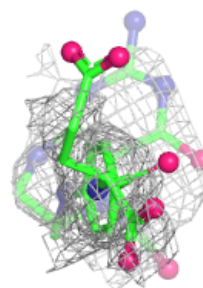
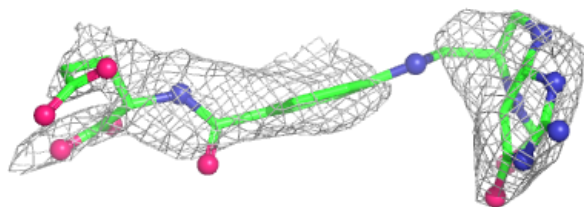
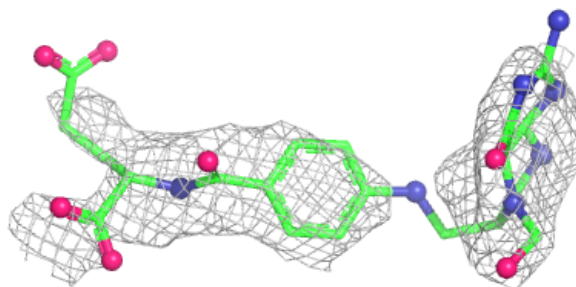
Electron density around PLG C 502:

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



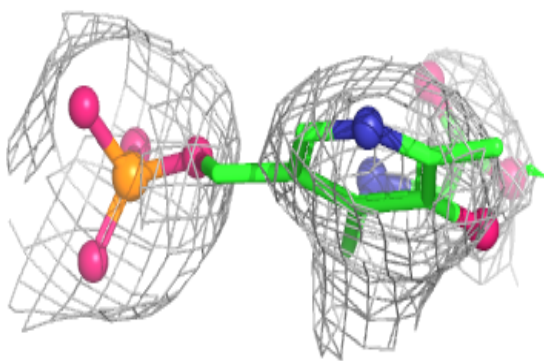
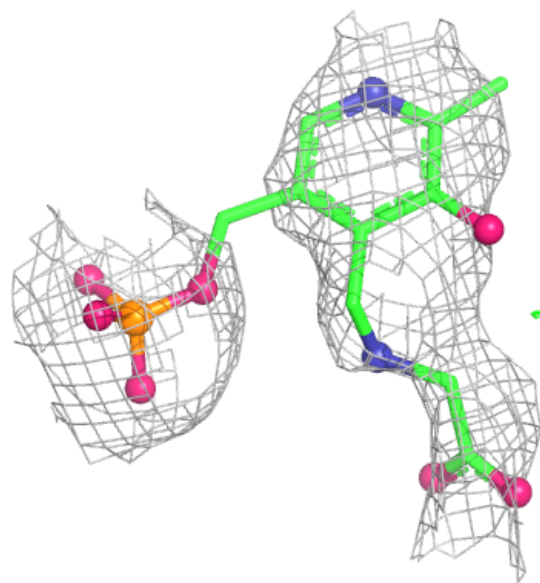
Electron density around THF B 601:

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



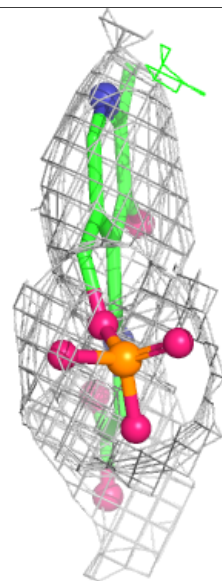
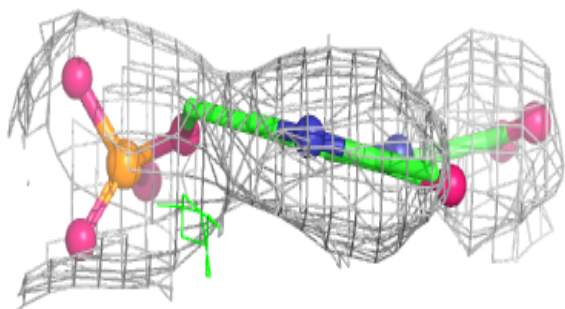
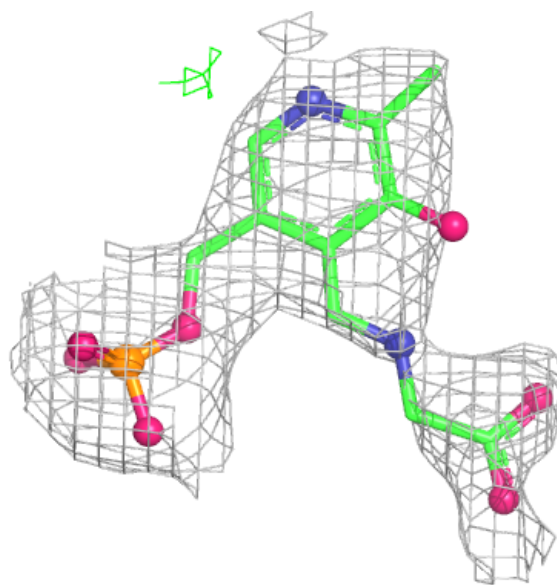
Electron density around PLG D 503:

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



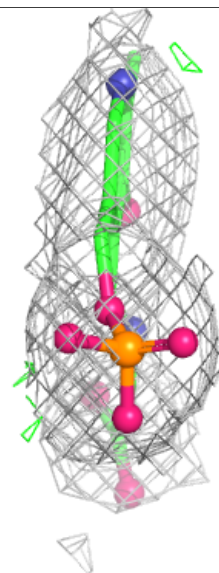
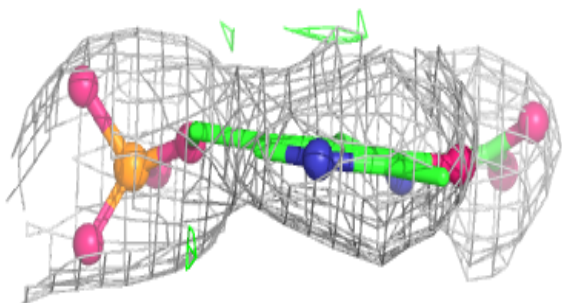
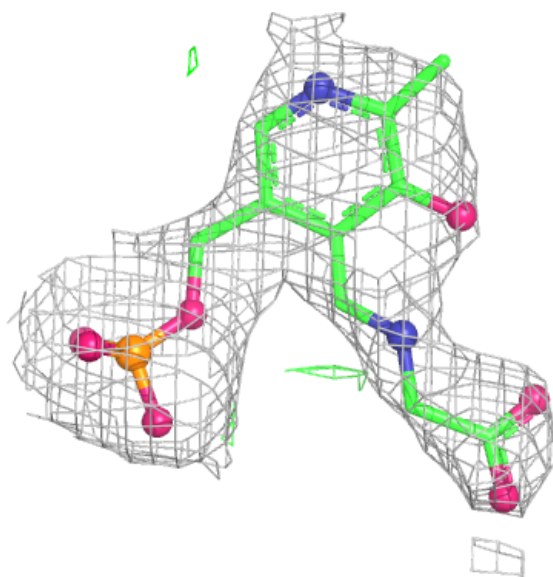
Electron density around PLG B 501:

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



Electron density around PLG A 500:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.