



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:45 AM UTC

PDB ID : 4C7R / pdb_00004c7r
Title : Inward facing conformation of the trimeric betaine transporter BetP in complex with lipids
Authors : Koshy, C.; Yildiz, O.; Ziegler, C.
Deposited on : 2013-09-24
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) : 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

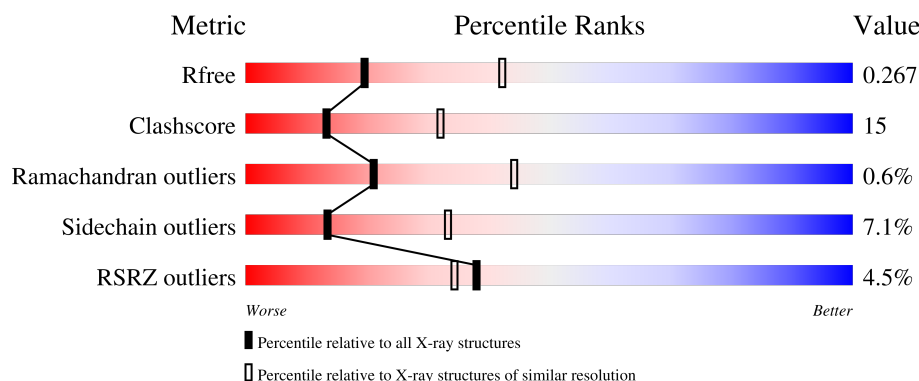
1 Overall quality at a glance i

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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	566	5% 65% 25% • 6%
1	B	566	5% 60% 25% • 12%
1	C	566	2% 61% 24% • 11%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12208 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.

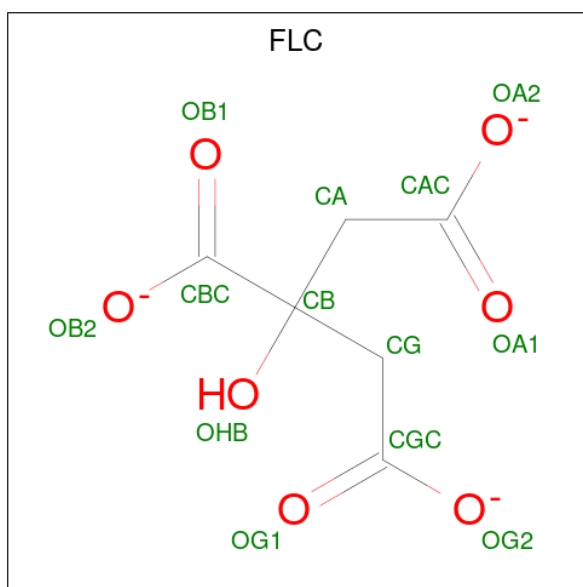
- Molecule 1 is a protein called GLYCINE BETAINES TRANSPORTER BETP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4057	2659	675	707	16			
1	B	497	Total	C	N	O	S	0	0	0
			3742	2473	595	658	16			
1	C	506	Total	C	N	O	S	0	0	0
			3827	2525	613	673	16			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	GLU	engineered mutation	UNP P54582
A	45	ALA	GLU	engineered mutation	UNP P54582
A	46	ALA	GLU	engineered mutation	UNP P54582
B	44	ALA	GLU	engineered mutation	UNP P54582
B	45	ALA	GLU	engineered mutation	UNP P54582
B	46	ALA	GLU	engineered mutation	UNP P54582
C	44	ALA	GLU	engineered mutation	UNP P54582
C	45	ALA	GLU	engineered mutation	UNP P54582
C	46	ALA	GLU	engineered mutation	UNP P54582

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).

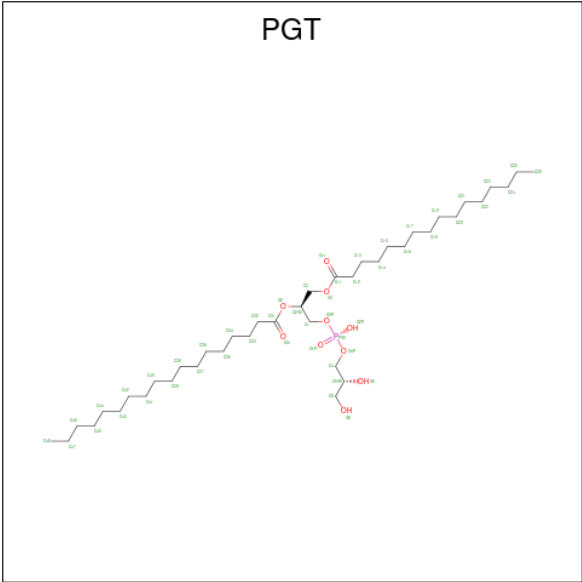


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		
2	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

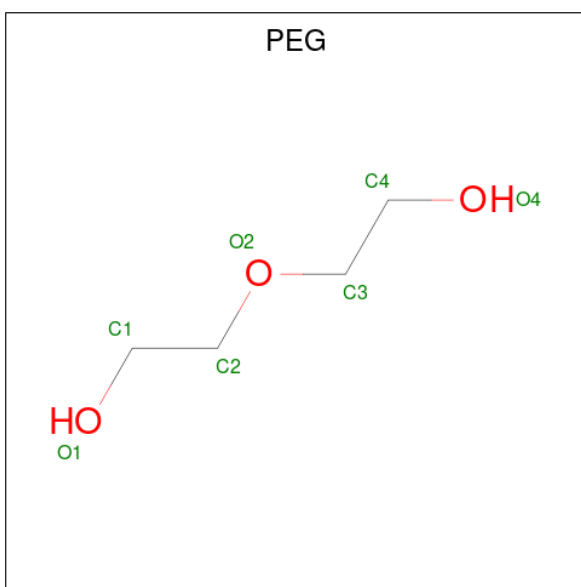
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	B	1	Total	Cl	0	0
			1	1		
3	C	3	Total	Cl	0	0
			3	3		

- Molecule 4 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



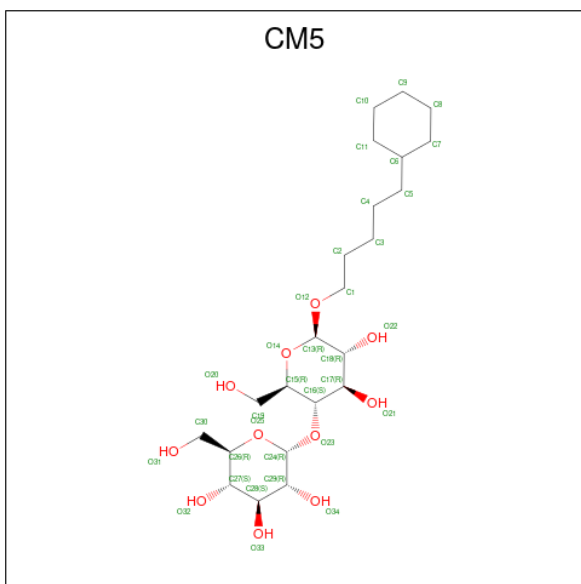
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			51	40	10	1		
4	A	1	Total	C	O	P	0	0
			51	40	10	1		
4	A	1	Total	C	O	P	0	0
			51	40	10	1		
4	A	1	Total	C			0	0
			18	18				
4	A	1	Total	C	O	P	0	0
			51	40	10	1		
4	B	1	Total	C	O	P	0	0
			51	40	10	1		
4	C	1	Total	C	O	P	0	0
			51	40	10	1		
4	C	1	Total	C	O	P	0	0
			51	40	10	1		
4	C	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			7	4	3		

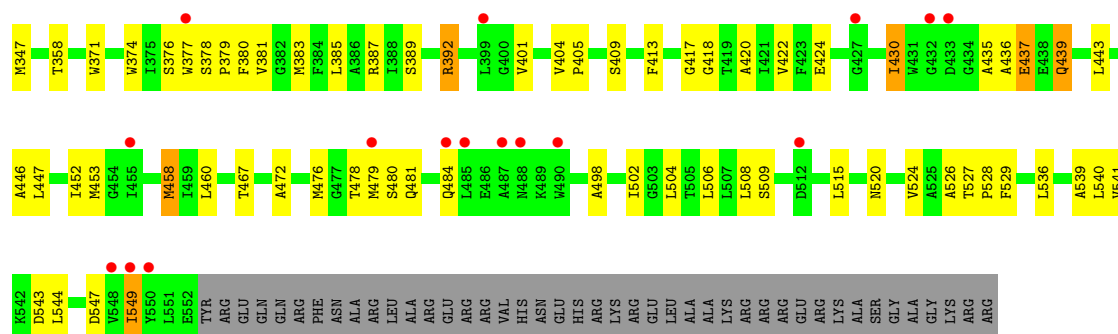
- Molecule 6 is 5-CYCLOHEXYL-1-PENTYL-BETA-D-MALTOSE (CCD ID: CM5) (formula: $C_{23}H_{42}O_{11}$).



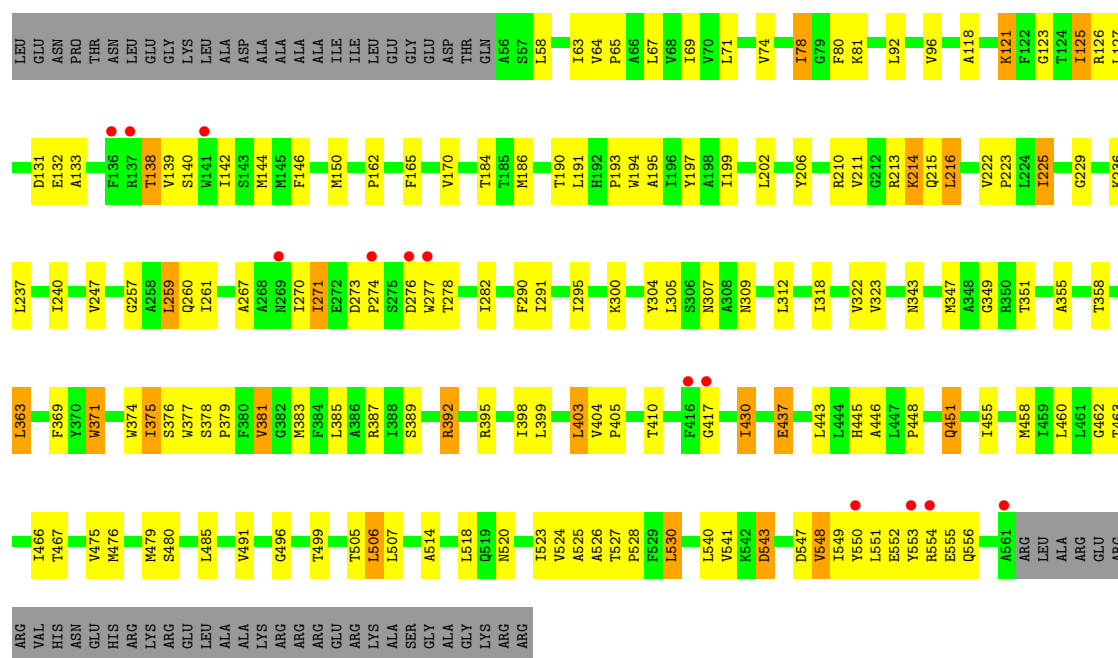
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			34	23	11		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	13	Total 13	O 13	0	0
7	B	23	Total 23	O 23	0	0
7	C	22	Total 22	O 22	0	0



● Molecule 1: GLYCINE BETAIN TRANSPORTER BETP



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	115.56Å 129.50Å 167.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.42 – 2.70 29.42 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.42-2.70) 99.8 (29.42-2.70)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.212 , 0.266 0.214 , 0.267	Depositor DCC
R_{free} test set	3678 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.4	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 74.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12208	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, FLC, CM5, PEG, PGT

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	0.31	0/4159	0.71	0/5661
1	B	0.32	0/3840	0.72	1/5241 (0.0%)
1	C	0.35	0/3927	0.74	1/5357 (0.0%)
All	All	0.33	0/11926	0.72	2/16259 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	GLN	N-CA-C	5.53	117.31	111.28
1	C	403	LEU	N-CA-C	5.12	116.94	111.36

There are no chirality outliers.

There are no planarity outliers.

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	4057	0	4098	116	0
1	B	3742	0	3775	103	0
1	C	3827	0	3852	122	0
2	A	13	0	5	0	0
2	B	13	0	5	3	0
2	C	26	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
4	A	222	0	347	28	0
4	B	51	0	78	5	0
4	C	153	0	234	15	0
5	B	7	0	10	0	0
6	C	34	0	42	3	0
7	A	13	0	0	0	0
7	B	23	0	0	2	0
7	C	22	0	0	0	0
All	All	12208	0	12456	365	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 15.

All (365) 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:A:252:CYS:HA	1:A:518:LEU:HD11	1.49	0.92
4:A:1589:PGT:H121	1:C:395:ARG:HD2	1.50	0.90
1:C:81:LYS:H	1:C:81:LYS:HD2	1.49	0.78
1:C:553:TYR:HA	1:C:556:GLN:HG2	1.67	0.76
4:A:1588:PGT:H342	4:A:1592:PGT:H131	1.67	0.76
4:A:1588:PGT:H251	4:A:1591:PGT:H321	1.67	0.75
1:A:147:ALA:HB1	1:A:310:MET:HE3	1.70	0.73
1:C:312:LEU:HB2	1:C:460:LEU:HD13	1.70	0.72
4:A:1588:PGT:H32	4:A:1588:PGT:H322	1.71	0.72
1:A:430:ILE:O	1:A:431:TRP:HB2	1.89	0.72
1:C:547:ASP:OD1	1:C:549:ILE:HG22	1.90	0.72
1:A:323:VAL:HG11	1:A:448:PRO:HD2	1.70	0.72
4:C:1565:PGT:H471	4:C:1565:PGT:H431	1.72	0.71
1:B:64:VAL:HB	1:B:65:PRO:HD3	1.71	0.71
4:A:1590:PGT:H322	1:C:395:ARG:HG2	1.70	0.71
1:B:259:LEU:HG	1:B:437:GLU:HG2	1.70	0.71
1:A:485:LEU:HD22	1:A:485:LEU:H	1.56	0.71
1:B:161:GLU:HB3	1:B:162:PRO:HD3	1.72	0.70
1:B:163:LEU:HD11	1:B:424:GLU:HG3	1.72	0.69
1:B:430:ILE:HG12	1:B:443:LEU:HA	1.74	0.69
1:A:290:PHE:CZ	1:A:496:GLY:HA3	2.28	0.68
1:A:120:SER:HB2	4:A:1589:PGT:H331	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LEU:HD13	1:B:101:TRP:CE2	2.30	0.66
1:B:225:ILE:HD11	1:B:234:LEU:HD23	1.78	0.66
1:A:92:LEU:HD13	1:A:520:ASN:HA	1.78	0.66
1:A:116:VAL:HG11	4:A:1590:PGT:H221	1.79	0.65
1:C:525:ALA:O	1:C:528:PRO:HD2	1.97	0.65
4:C:1567:PGT:H151	6:C:1568:CM5:H21A	1.77	0.65
1:A:225:ILE:HG23	1:A:229:GLY:HA3	1.79	0.65
1:A:379:PRO:HG3	1:A:529:PHE:CZ	2.32	0.64
4:A:1589:PGT:H322	4:A:1590:PGT:H121	1.78	0.64
1:C:225:ILE:HG23	1:C:229:GLY:HA3	1.78	0.64
1:C:225:ILE:HD11	6:C:1568:CM5:H51	1.77	0.64
4:A:1589:PGT:H221	1:C:191:LEU:HD21	1.80	0.64
1:C:193:PRO:HB3	1:C:374:TRP:CD1	2.33	0.64
1:A:122:PHE:HB3	1:A:544:LEU:HD23	1.80	0.63
4:A:1589:PGT:H5	4:A:1592:PGT:H31	1.80	0.63
1:B:223:PRO:HG3	1:B:543:ASP:OD1	1.98	0.63
1:A:355:ALA:O	1:A:358:THR:HB	1.97	0.63
1:C:150:MET:O	2:C:1001:FLC:HG1	1.97	0.63
1:C:506:LEU:HD23	1:C:518:LEU:HD12	1.80	0.62
1:A:325:PRO:HB2	1:A:328:SER:HB2	1.81	0.62
1:A:452:ILE:HG13	1:A:453:MET:N	2.14	0.62
1:B:306:SER:O	1:B:310:MET:HG2	1.99	0.62
1:A:399:LEU:HD11	4:A:1588:PGT:H182	1.83	0.61
1:A:559:PHE:HE1	1:A:563:LEU:HD12	1.66	0.61
4:A:1589:PGT:H121	1:C:395:ARG:CD	2.27	0.60
1:B:319:PHE:O	1:B:323:VAL:HG22	2.01	0.60
1:B:228:LYS:H	1:B:228:LYS:HD3	1.66	0.60
1:B:261:ILE:HG13	1:B:458:MET:HG2	1.83	0.60
4:A:1589:PGT:H162	1:C:399:LEU:HD21	1.83	0.60
1:B:452:ILE:H	1:B:452:ILE:HD12	1.67	0.59
1:C:64:VAL:HB	1:C:65:PRO:HD3	1.84	0.59
4:A:1590:PGT:C32	1:C:395:ARG:HG2	2.33	0.59
4:A:1588:PGT:H352	4:A:1589:PGT:H392	1.85	0.59
4:C:1565:PGT:H471	4:C:1565:PGT:H371	1.84	0.59
1:A:581:LYS:HG3	1:A:582:ARG:N	2.16	0.59
1:C:383:MET:SD	1:C:475:VAL:HG13	2.43	0.59
1:A:119:ALA:HA	4:A:1588:PGT:H132	1.85	0.59
4:A:1589:PGT:H31	4:A:1589:PGT:H342	1.84	0.59
1:C:150:MET:O	2:C:1001:FLC:HA1	2.03	0.58
1:B:98:ASN:HD22	1:B:98:ASN:N	2.00	0.58
1:C:309:ASN:HD21	1:C:467:THR:HG21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:VAL:HG21	1:B:504:LEU:HD13	1.85	0.58
1:C:186:MET:HE1	1:C:410:THR:OG1	2.03	0.58
1:A:547:ASP:OD2	1:A:549:ILE:HG22	2.04	0.58
4:B:1554:PGT:H241	4:B:1554:PGT:H201	1.85	0.58
1:A:64:VAL:HB	1:A:65:PRO:HD3	1.86	0.58
1:B:376:SER:HB3	1:B:526:ALA:HB2	1.85	0.57
1:C:463:THR:O	1:C:467:THR:HG23	2.04	0.57
1:B:404:VAL:HB	1:B:405:PRO:HD3	1.86	0.57
1:C:215:GLN:HE22	1:C:387:ARG:HD2	1.68	0.57
1:C:291:ILE:O	1:C:295:ILE:HG12	2.04	0.57
1:B:236:LYS:O	1:B:240:ILE:HG13	2.04	0.57
1:C:165:PHE:CE2	1:C:184:THR:HG22	2.39	0.57
1:A:287:THR:O	1:A:291:ILE:HG13	2.05	0.57
1:A:323:VAL:CG1	1:A:448:PRO:HD2	2.35	0.57
1:C:125:ILE:HG12	1:C:549:ILE:CG2	2.35	0.57
1:A:114:ILE:HG13	1:A:398:ILE:HD13	1.85	0.57
1:B:478:THR:HG23	1:B:484:GLN:O	2.04	0.57
1:C:92:LEU:HG	1:C:520:ASN:CG	2.29	0.57
1:A:430:ILE:HG22	1:A:431:TRP:N	2.20	0.56
1:B:150:MET:O	2:B:1001:FLC:HG2	2.05	0.56
1:B:202:LEU:HD23	1:B:540:LEU:HD21	1.86	0.56
1:A:559:PHE:CE1	1:A:563:LEU:HD12	2.40	0.56
1:B:207:SER:O	1:B:213:ARG:HB2	2.05	0.56
1:B:547:ASP:OD2	1:B:549:ILE:HG22	2.04	0.56
1:C:150:MET:HE1	4:C:1565:PGT:H472	1.86	0.56
1:B:520:ASN:O	1:B:524:VAL:HG23	2.05	0.56
4:A:1592:PGT:C32	4:A:1592:PGT:H11	2.36	0.56
1:B:312:LEU:HB2	1:B:460:LEU:HD13	1.87	0.56
1:C:202:LEU:HD23	1:C:540:LEU:HD21	1.88	0.55
1:B:113:PHE:HA	4:B:1554:PGT:H151	1.88	0.55
1:B:307:ASN:O	1:B:311:VAL:HG12	2.06	0.55
1:A:257:GLY:O	1:A:261:ILE:HG22	2.05	0.55
1:A:537:MET:O	1:A:541:VAL:HG23	2.06	0.55
1:B:319:PHE:CD2	1:B:453:MET:HG3	2.42	0.55
1:C:355:ALA:O	1:C:358:THR:HG22	2.06	0.55
1:C:259:LEU:HD22	1:C:437:GLU:HG2	1.88	0.55
1:B:160:THR:HG23	1:B:439:GLN:HE22	1.71	0.54
1:B:193:PRO:HB3	1:B:374:TRP:CD1	2.41	0.54
1:C:257:GLY:O	1:C:261:ILE:HG22	2.07	0.54
1:A:140:SER:O	1:A:144:MET:HG3	2.08	0.54
1:A:527:THR:HB	1:A:528:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:SER:O	1:A:392:ARG:HB2	2.08	0.54
1:A:228:LYS:H	1:A:228:LYS:HD3	1.74	0.53
1:A:472:ALA:O	1:A:476:MET:HG3	2.08	0.53
1:C:215:GLN:NE2	1:C:387:ARG:HD2	2.23	0.53
1:C:381:VAL:O	1:C:385:LEU:HG	2.09	0.53
1:B:198:ALA:HB2	1:B:401:VAL:HG11	1.91	0.53
1:B:228:LYS:HD3	1:B:228:LYS:N	2.23	0.53
1:B:380:PHE:CD1	1:B:380:PHE:C	2.86	0.53
1:C:63:ILE:HG12	1:C:480:SER:HB2	1.90	0.53
1:C:223:PRO:HG3	1:C:543:ASP:OD1	2.09	0.53
1:C:132:GLU:HG3	1:C:133:ALA:H	1.74	0.53
1:A:186:MET:HE1	1:A:410:THR:OG1	2.09	0.52
1:C:369:PHE:HA	1:C:523:ILE:HD11	1.89	0.52
1:B:243:ILE:HG12	1:B:479:MET:HE2	1.92	0.52
1:A:423:PHE:CD2	1:A:430:ILE:HD13	2.45	0.52
1:A:65:PRO:O	1:A:69:ILE:HG12	2.09	0.52
1:B:333:LEU:HB2	1:B:334:PRO:CD	2.40	0.52
4:A:1589:PGT:H461	4:A:1592:PGT:H261	1.90	0.52
1:B:381:VAL:O	1:B:385:LEU:HG	2.09	0.52
4:C:1567:PGT:C4	4:C:1567:PGT:H12	2.39	0.52
1:C:247:VAL:HB	1:C:476:MET:HE1	1.92	0.52
1:C:259:LEU:HD13	1:C:437:GLU:HG2	1.92	0.52
1:A:297:GLY:O	1:A:300:LYS:HG2	2.09	0.51
1:A:121:LYS:O	1:A:121:LYS:HD3	2.10	0.51
1:A:333:LEU:HB2	1:A:334:PRO:CD	2.39	0.51
1:C:121:LYS:HB3	1:C:550:TYR:HD2	1.75	0.51
1:C:455:ILE:HA	1:C:458:MET:HE2	1.93	0.51
1:B:63:ILE:HG12	1:B:480:SER:HB2	1.93	0.51
1:B:230:ALA:HA	1:B:235:GLY:HA3	1.93	0.51
1:A:193:PRO:HB3	1:A:374:TRP:CD1	2.46	0.51
4:A:1589:PGT:H232	1:C:191:LEU:HD11	1.93	0.51
1:C:549:ILE:O	1:C:552:GLU:HB2	2.10	0.51
1:A:247:VAL:HG23	1:A:499:THR:HA	1.93	0.51
1:A:530:LEU:O	1:A:534:ILE:HG13	2.12	0.50
1:B:148:ALA:O	2:B:1001:FLC:HA1	2.12	0.50
1:A:106:PHE:HA	1:A:109:VAL:HB	1.93	0.50
4:A:1589:PGT:C12	1:C:395:ARG:HD2	2.34	0.50
1:C:351:THR:HA	1:C:363:LEU:HD21	1.93	0.50
1:B:159:THR:HG23	1:B:420:ALA:HB2	1.93	0.50
1:B:80:PHE:O	1:B:81:LYS:C	2.55	0.50
1:C:451:GLN:H	1:C:451:GLN:NE2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:PRO:HG3	1:B:529:PHE:CZ	2.47	0.49
1:C:125:ILE:HG22	1:C:126:ARG:N	2.26	0.49
1:A:138:THR:HA	1:A:392:ARG:NH2	2.27	0.49
1:B:70:VAL:HG11	1:B:498:ALA:HB1	1.94	0.49
1:C:278:THR:O	1:C:282:ILE:HG13	2.12	0.49
1:A:430:ILE:O	1:A:431:TRP:CB	2.56	0.49
1:A:430:ILE:HD12	1:A:430:ILE:N	2.28	0.49
1:B:200:VAL:HG21	1:B:378:SER:HB2	1.95	0.49
1:C:273:ASP:OD1	1:C:274:PRO:HD2	2.11	0.49
1:B:62:VAL:HG12	1:B:236:LYS:HB3	1.95	0.49
1:B:270:ILE:O	1:B:271:ILE:HD12	2.12	0.49
1:B:59:ASN:O	1:B:62:VAL:HG22	2.12	0.49
1:A:202:LEU:HD23	1:A:540:LEU:HD21	1.93	0.49
1:A:330:LEU:HD13	1:B:101:TRP:NE1	2.28	0.49
1:A:301:GLY:HA2	1:A:304:TYR:CE2	2.48	0.49
1:B:111:VAL:O	1:B:115:VAL:HG13	2.13	0.49
1:A:264:GLY:HA3	1:A:441:PHE:CZ	2.48	0.49
1:C:74:VAL:HA	1:C:505:THR:HG21	1.94	0.49
1:A:431:TRP:HA	1:A:439:GLN:HE21	1.76	0.48
1:A:568:ARG:HD3	1:C:548:VAL:CG2	2.44	0.48
1:C:323:VAL:CG1	1:C:448:PRO:HD2	2.42	0.48
1:B:389:SER:O	1:B:392:ARG:HB2	2.13	0.48
1:C:290:PHE:CE2	1:C:496:GLY:HA3	2.48	0.48
1:B:257:GLY:O	1:B:261:ILE:HG22	2.13	0.48
1:B:452:ILE:HD12	1:B:452:ILE:N	2.28	0.48
1:C:132:GLU:CG	1:C:133:ALA:N	2.77	0.48
1:C:376:SER:HB3	1:C:526:ALA:HB2	1.94	0.48
1:B:221:PHE:CE1	1:B:536:LEU:HD13	2.49	0.48
1:A:290:PHE:CZ	1:A:493:ALA:HA	2.49	0.48
1:B:80:PHE:CD1	1:B:80:PHE:N	2.81	0.48
1:B:98:ASN:N	1:B:98:ASN:ND2	2.62	0.48
1:A:163:LEU:HG	1:A:420:ALA:HB1	1.96	0.48
1:A:423:PHE:HD2	1:A:430:ILE:HD13	1.79	0.48
1:B:266:SER:OG	1:B:274:PRO:HD3	2.13	0.48
1:B:278:THR:O	1:B:282:ILE:HG13	2.13	0.48
1:C:65:PRO:HB2	1:C:240:ILE:HD13	1.96	0.48
1:C:375:ILE:HD12	1:C:530:LEU:HA	1.96	0.48
1:A:92:LEU:HD22	1:A:520:ASN:CG	2.39	0.48
1:A:300:LYS:HG3	1:A:301:GLY:N	2.29	0.48
1:B:170:VAL:HG13	1:B:171:PRO:HD2	1.94	0.48
1:B:409:SER:O	1:B:413:PHE:HD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ALA:HB1	1:C:445:HIS:CE1	2.49	0.48
1:C:430:ILE:HG12	1:C:443:LEU:HA	1.96	0.48
1:C:462:GLY:O	1:C:466:ILE:HG13	2.13	0.48
1:A:444:LEU:O	1:A:450:GLY:HA3	2.14	0.47
4:C:1567:PGT:H42	4:C:1567:PGT:C11	2.44	0.47
1:C:214:LYS:HZ3	1:C:214:LYS:HB2	1.79	0.47
1:C:270:ILE:HG22	1:C:270:ILE:O	2.14	0.47
1:B:206:TYR:CE2	1:B:543:ASP:HB3	2.49	0.47
1:C:71:LEU:O	1:C:74:VAL:HG22	2.14	0.47
1:C:118:ALA:O	1:C:395:ARG:HD3	2.13	0.47
1:C:140:SER:O	1:C:144:MET:HG3	2.14	0.47
1:A:81:LYS:H	1:A:81:LYS:HD2	1.78	0.47
4:A:1589:PGT:H361	4:A:1589:PGT:H32	1.96	0.47
1:B:150:MET:O	2:B:1001:FLC:HA2	2.13	0.47
1:C:378:SER:OG	1:C:379:PRO:HD3	2.14	0.47
1:B:527:THR:HB	1:B:528:PRO:HD3	1.97	0.47
1:B:225:ILE:HG23	1:B:229:GLY:HA3	1.95	0.47
1:B:430:ILE:HD11	1:B:446:ALA:HB2	1.97	0.47
1:C:121:LYS:HB3	1:C:550:TYR:CD2	2.50	0.47
1:A:278:THR:O	1:A:282:ILE:HG13	2.15	0.47
1:A:428:GLU:O	1:A:430:ILE:HD12	2.15	0.47
1:A:581:LYS:O	1:A:585:GLU:HB2	2.14	0.47
1:B:218:SER:HB3	1:B:235:GLY:O	2.14	0.47
1:C:300:LYS:HD2	1:C:300:LYS:C	2.39	0.47
1:A:163:LEU:HD13	1:A:431:TRP:HE3	1.80	0.47
1:A:430:ILE:CG2	1:A:431:TRP:N	2.78	0.47
1:B:187:PHE:CD1	1:B:347:MET:HE3	2.50	0.46
1:B:203:ALA:HA	1:B:540:LEU:HD13	1.97	0.46
1:C:260:GLN:HA	1:C:437:GLU:HB3	1.98	0.46
4:C:1566:PGT:H32	4:C:1566:PGT:H42	1.96	0.46
1:C:190:THR:O	1:C:193:PRO:HD2	2.15	0.46
1:A:261:ILE:HG21	1:A:282:ILE:HG21	1.98	0.46
1:A:353:MET:HE3	1:A:353:MET:HB3	1.77	0.46
1:C:309:ASN:ND2	1:C:467:THR:HG21	2.30	0.46
1:C:527:THR:HB	1:C:528:PRO:HD3	1.97	0.46
1:C:404:VAL:HB	1:C:405:PRO:HD3	1.98	0.46
1:B:226:GLY:HA3	1:B:228:LYS:NZ	2.31	0.46
1:C:138:THR:O	1:C:142:ILE:HG13	2.14	0.46
1:C:206:TYR:CE2	1:C:210:ARG:HG2	2.51	0.46
1:C:430:ILE:HD12	1:C:430:ILE:HA	1.73	0.46
1:A:445:HIS:C	1:A:447:LEU:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:TYR:O	1:C:307:ASN:HB2	2.16	0.46
1:A:232:GLY:O	1:A:236:LYS:HG2	2.16	0.46
1:C:132:GLU:CG	1:C:133:ALA:H	2.29	0.46
4:C:1567:PGT:C35	4:C:1567:PGT:C31	2.94	0.46
1:A:236:LYS:O	1:A:240:ILE:HG13	2.16	0.46
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.76	0.46
1:A:228:LYS:H	1:A:228:LYS:CD	2.29	0.45
1:A:222:VAL:N	1:A:223:PRO:CD	2.79	0.45
1:B:333:LEU:HB2	1:B:334:PRO:HD2	1.97	0.45
1:C:206:TYR:O	1:C:210:ARG:HB3	2.16	0.45
1:C:270:ILE:O	1:C:271:ILE:HG13	2.16	0.45
1:A:63:ILE:HG12	1:A:480:SER:HB2	1.99	0.45
1:B:92:LEU:HD13	1:B:92:LEU:C	2.42	0.45
1:B:81:LYS:HG3	1:B:509:SER:HA	1.98	0.45
1:A:380:PHE:HA	1:A:475:VAL:HG11	1.98	0.45
1:A:254:LEU:HD22	1:A:465:PHE:CE2	2.51	0.45
1:A:520:ASN:O	1:A:524:VAL:HG23	2.17	0.45
1:A:493:ALA:O	1:A:497:VAL:HG23	2.17	0.45
1:B:323:VAL:HG23	1:B:447:LEU:HD13	1.99	0.45
1:B:418:GLY:O	1:B:422:VAL:HG23	2.17	0.45
1:A:488:ASN:HD22	1:A:491:VAL:HG23	1.82	0.44
4:A:1592:PGT:H381	4:A:1592:PGT:H412	1.80	0.44
1:C:138:THR:HA	1:C:392:ARG:HH22	1.83	0.44
1:C:276:ASP:C	1:C:278:THR:H	2.25	0.44
1:C:318:ILE:O	1:C:322:VAL:HG23	2.17	0.44
1:C:507:LEU:HD23	1:C:514:ALA:HB1	1.99	0.44
1:B:243:ILE:O	1:B:247:VAL:HG23	2.17	0.44
1:A:150:MET:HG2	1:A:408:VAL:HG11	1.98	0.44
1:B:378:SER:OG	1:B:379:PRO:HD3	2.17	0.44
1:B:424:GLU:HG2	7:B:2023:HOH:O	2.17	0.44
1:A:260:GLN:HG2	1:A:461:LEU:HD11	2.00	0.44
1:C:343:ASN:O	1:C:347:MET:HG3	2.17	0.44
1:A:150:MET:HE2	1:A:408:VAL:HG13	2.00	0.44
1:A:239:ASP:O	1:A:243:ILE:HG13	2.17	0.44
1:C:80:PHE:O	1:C:81:LYS:C	2.60	0.44
1:C:194:TRP:CE3	1:C:197:TYR:HD2	2.35	0.44
1:C:195:ALA:O	1:C:199:ILE:HG13	2.18	0.44
1:C:236:LYS:HA	1:C:236:LYS:HD3	1.85	0.44
1:C:318:ILE:HD11	4:C:1565:PGT:H412	1.98	0.44
1:A:583:ARG:HE	1:A:583:ARG:HA	1.83	0.44
1:A:584:ARG:CD	1:A:584:ARG:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:O	1:A:247:VAL:HG12	2.18	0.44
1:A:261:ILE:CG2	1:A:282:ILE:HG21	2.47	0.43
1:C:323:VAL:HG11	1:C:448:PRO:HD2	2.00	0.43
1:A:218:SER:HB3	1:A:235:GLY:O	2.18	0.43
1:C:213:ARG:NH2	1:C:543:ASP:OD2	2.50	0.43
1:C:305:LEU:CB	1:C:467:THR:HG22	2.48	0.43
1:A:488:ASN:ND2	1:A:491:VAL:HG23	2.33	0.43
1:B:162:PRO:HG2	1:B:417:GLY:HA3	2.00	0.43
1:C:222:VAL:N	1:C:223:PRO:CD	2.81	0.43
1:A:371:TRP:CE3	1:A:371:TRP:CA	3.01	0.43
1:A:436:ALA:HA	1:A:439:GLN:OE1	2.18	0.43
1:B:222:VAL:HB	1:B:223:PRO:HD3	1.99	0.43
4:B:1554:PGT:H192	4:B:1554:PGT:H222	1.58	0.43
1:A:475:VAL:O	1:A:479:MET:HB2	2.19	0.43
1:A:584:ARG:H	1:A:584:ARG:HD3	1.83	0.43
1:B:316:LEU:HD23	1:B:316:LEU:HA	1.83	0.43
1:C:74:VAL:O	1:C:78:ILE:HB	2.19	0.43
1:C:371:TRP:N	1:C:371:TRP:CE3	2.86	0.43
1:C:389:SER:O	1:C:392:ARG:HB2	2.19	0.43
4:A:1589:PGT:H222	1:C:403:LEU:HD21	1.99	0.43
1:B:64:VAL:O	1:B:68:VAL:HG23	2.18	0.43
1:A:202:LEU:HD11	1:A:394:ILE:HG12	2.00	0.43
1:A:220:ALA:O	1:A:539:ALA:HB1	2.19	0.43
4:A:1592:PGT:H222	4:B:1554:PGT:H401	2.01	0.43
1:B:58:LEU:HD23	1:B:481:GLN:HG2	2.00	0.43
1:C:125:ILE:HG12	1:C:549:ILE:HG23	2.00	0.43
1:C:371:TRP:N	1:C:371:TRP:HE3	2.15	0.43
1:C:65:PRO:O	1:C:69:ILE:HG12	2.19	0.43
1:C:162:PRO:CG	1:C:417:GLY:HA3	2.49	0.43
1:C:121:LYS:O	1:C:121:LYS:HD3	2.19	0.43
1:A:261:ILE:O	1:A:458:MET:HE1	2.19	0.42
1:C:92:LEU:O	1:C:96:VAL:HG23	2.18	0.42
1:C:290:PHE:CZ	1:C:496:GLY:HA3	2.54	0.42
1:C:443:LEU:C	1:C:443:LEU:HD23	2.44	0.42
1:C:551:LEU:O	1:C:555:GLU:HB2	2.18	0.42
4:C:1565:PGT:H431	4:C:1565:PGT:H402	1.63	0.42
1:B:59:ASN:HD21	1:B:236:LYS:NZ	2.17	0.42
1:B:314:ALA:O	1:B:318:ILE:HD13	2.19	0.42
1:C:541:VAL:HG11	4:C:1567:PGT:H411	2.01	0.42
1:A:502:ILE:O	1:A:506:LEU:HG	2.19	0.42
1:B:115:VAL:HG21	4:B:1554:PGT:H432	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:PHE:CE2	1:A:496:GLY:HA3	2.55	0.42
1:B:239:ASP:O	1:B:243:ILE:HG13	2.19	0.42
1:A:329:ILE:HD13	1:A:415:ILE:HA	2.00	0.42
1:B:224:LEU:HD22	1:B:539:ALA:HB2	2.00	0.42
1:B:502:ILE:O	1:B:506:LEU:HD13	2.20	0.42
1:C:211:VAL:O	1:C:211:VAL:HG12	2.19	0.42
1:C:520:ASN:O	1:C:524:VAL:HG23	2.19	0.42
1:A:333:LEU:HB2	1:A:334:PRO:HD3	2.00	0.42
1:A:404:VAL:HB	1:A:405:PRO:HD3	2.00	0.42
1:B:258:ALA:HA	1:B:261:ILE:CG2	2.50	0.42
1:B:258:ALA:HA	1:B:261:ILE:HG22	2.01	0.42
1:C:138:THR:HA	1:C:392:ARG:NH2	2.34	0.42
1:B:472:ALA:O	1:B:476:MET:HG3	2.19	0.42
1:C:216:LEU:HD12	1:C:216:LEU:HA	1.78	0.42
1:A:371:TRP:CE3	1:A:371:TRP:HA	2.55	0.42
1:A:393:SER:OG	1:A:396:GLU:HB2	2.19	0.42
1:B:177:ASN:HA	7:B:2008:HOH:O	2.19	0.42
1:A:250:THR:HB	1:A:499:THR:HG21	2.02	0.41
1:B:107:GLY:HA2	1:B:110:PHE:CD2	2.55	0.41
4:A:1589:PGT:H263	4:A:1589:PGT:H231	1.83	0.41
1:B:308:ALA:O	1:B:309:ASN:C	2.63	0.41
1:B:335:GLY:HA2	1:C:349:GLY:O	2.20	0.41
1:A:77:GLY:HA3	1:A:505:THR:CG2	2.50	0.41
1:A:283:VAL:O	1:A:287:THR:HB	2.20	0.41
1:A:343:ASN:HB2	1:A:347:MET:HE2	2.01	0.41
1:A:372:ALA:HB1	1:A:523:ILE:HA	2.03	0.41
1:A:455:ILE:HA	1:A:458:MET:HG3	2.03	0.41
1:B:66:ALA:O	1:B:70:VAL:HG23	2.20	0.41
4:C:1567:PGT:C6	6:C:1568:CM5:H11	2.51	0.41
1:A:119:ALA:HA	4:A:1588:PGT:C13	2.51	0.41
1:C:118:ALA:HB2	1:C:398:ILE:HD12	2.02	0.41
1:C:206:TYR:OH	1:C:547:ASP:HB2	2.21	0.41
1:B:504:LEU:O	1:B:508:LEU:HG	2.20	0.41
1:C:123:GLY:HA3	1:C:395:ARG:NH1	2.36	0.41
1:A:163:LEU:HD13	1:A:431:TRP:CE3	2.56	0.41
1:A:265:LEU:HD13	1:A:271:ILE:HD12	2.02	0.41
1:A:272:GLU:C	1:A:274:PRO:HD3	2.45	0.41
1:A:371:TRP:CE3	1:A:371:TRP:N	2.89	0.41
1:B:435:ALA:O	1:B:436:ALA:C	2.63	0.41
1:C:485:LEU:HD22	1:C:485:LEU:H	1.85	0.41
4:C:1565:PGT:H171	4:C:1565:PGT:H142	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:MET:O	1:B:387:ARG:HG3	2.21	0.41
4:C:1565:PGT:H322	4:C:1565:PGT:H2	1.73	0.41
4:A:1588:PGT:H352	4:A:1589:PGT:C39	2.51	0.40
1:B:343:ASN:O	1:B:347:MET:HG3	2.21	0.40
1:C:58:LEU:HD11	1:C:491:VAL:HG21	2.03	0.40
4:C:1565:PGT:H421	4:C:1566:PGT:H481	2.02	0.40
1:B:122:PHE:CD1	1:B:544:LEU:HB3	2.57	0.40
1:A:417:GLY:O	1:A:421:ILE:HG13	2.21	0.40
1:A:452:ILE:HG13	1:A:453:MET:H	1.87	0.40
1:B:146:PHE:C	1:B:148:ALA:N	2.79	0.40
1:B:224:LEU:HD13	1:B:539:ALA:HA	2.04	0.40
1:B:430:ILE:O	1:B:430:ILE:HG23	2.22	0.40
1:C:247:VAL:HG23	1:C:499:THR:OG1	2.22	0.40
1:C:430:ILE:HD11	1:C:446:ALA:HB2	2.02	0.40
1:C:550:TYR:CD1	1:C:550:TYR:C	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	529/566 (94%)	496 (94%)	28 (5%)	5 (1%)	14	35
1	B	495/566 (88%)	458 (92%)	35 (7%)	2 (0%)	30	54
1	C	504/566 (89%)	476 (94%)	26 (5%)	2 (0%)	30	54
All	All	1528/1698 (90%)	1430 (94%)	89 (6%)	9 (1%)	21	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	583	ARG
1	A	431	TRP

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Mol	Chain	Res	Type
1	B	81	LYS
1	A	585	GLU
1	C	131	ASP
1	A	485	LEU
1	B	272	GLU
1	A	448	PRO
1	C	125	ILE

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	415/439 (94%)	385 (93%)	30 (7%)	13	32
1	B	385/439 (88%)	360 (94%)	25 (6%)	15	37
1	C	393/439 (90%)	363 (92%)	30 (8%)	12	30
All	All	1193/1317 (91%)	1108 (93%)	85 (7%)	13	33

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LEU
1	A	137	ARG
1	A	139	VAL
1	A	163	LEU
1	A	214	LYS
1	A	216	LEU
1	A	225	ILE
1	A	228	LYS
1	A	247	VAL
1	A	270	ILE
1	A	287	THR
1	A	295	ILE
1	A	302	ILE
1	A	316	LEU
1	A	328	SER

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Mol	Chain	Res	Type
1	A	358	THR
1	A	363	LEU
1	A	371	TRP
1	A	399	LEU
1	A	402	LEU
1	A	437	GLU
1	A	439	GLN
1	A	458	MET
1	A	479	MET
1	A	485	LEU
1	A	504	LEU
1	A	543	ASP
1	A	549	ILE
1	A	563	LEU
1	A	569	VAL
1	B	67	LEU
1	B	80	PHE
1	B	98	ASN
1	B	108	THR
1	B	115	VAL
1	B	131	ASP
1	B	224	LEU
1	B	225	ILE
1	B	228	LYS
1	B	261	ILE
1	B	271	ILE
1	B	302	ILE
1	B	311	VAL
1	B	327	VAL
1	B	358	THR
1	B	371	TRP
1	B	377	TRP
1	B	392	ARG
1	B	430	ILE
1	B	437	GLU
1	B	458	MET
1	B	467	THR
1	B	515	LEU
1	B	541	VAL
1	B	549	ILE
1	C	67	LEU
1	C	78	ILE

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Mol	Chain	Res	Type
1	C	121	LYS
1	C	127	LEU
1	C	138	THR
1	C	139	VAL
1	C	146	PHE
1	C	170	VAL
1	C	214	LYS
1	C	216	LEU
1	C	225	ILE
1	C	237	LEU
1	C	259	LEU
1	C	271	ILE
1	C	277	TRP
1	C	363	LEU
1	C	371	TRP
1	C	375	ILE
1	C	377	TRP
1	C	381	VAL
1	C	392	ARG
1	C	430	ILE
1	C	437	GLU
1	C	451	GLN
1	C	479	MET
1	C	506	LEU
1	C	530	LEU
1	C	543	ASP
1	C	548	VAL
1	C	554	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	439	GLN
1	A	445	HIS
1	A	557	GLN
1	A	571	ASN
1	A	573	HIS
1	B	59	ASN
1	B	98	ASN
1	B	215	GLN
1	B	303	GLN
1	B	346	GLN

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Mol	Chain	Res	Type
1	B	439	GLN
1	B	451	GLN
1	B	482	HIS
1	B	488	ASN
1	B	517	ASN
1	C	215	GLN
1	C	481	GLN
1	C	560	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 5 are monoatomic - leaving 15 for Mogul analysis.

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	$\# Z > 2$
4	PGT	A	1591	-	17,17,50	0.23	0	16,16,56	0.61	0
2	FLC	C	1001	-	12,12,12	1.22	1 (8%)	17,17,17	1.18	1 (5%)
5	PEG	B	1555	-	6,6,6	0.46	0	5,5,5	0.25	0
4	PGT	A	1592	-	50,50,50	0.93	2 (4%)	53,56,56	1.04	3 (5%)
4	PGT	C	1565	-	50,50,50	0.92	2 (4%)	53,56,56	1.05	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGT	B	1554	-	50,50,50	0.94	2 (4%)	53,56,56	0.99	3 (5%)
2	FLC	B	1001	-	12,12,12	1.21	1 (8%)	17,17,17	1.17	1 (5%)
4	PGT	C	1567	-	50,50,50	0.94	2 (4%)	53,56,56	0.99	3 (5%)
2	FLC	A	1001	-	12,12,12	1.14	0	17,17,17	1.03	1 (5%)
6	CM5	C	1568	-	36,36,36	0.40	0	49,49,49	0.78	1 (2%)
4	PGT	A	1589	-	50,50,50	0.97	2 (4%)	53,56,56	0.98	2 (3%)
4	PGT	A	1588	-	50,50,50	0.94	2 (4%)	53,56,56	1.08	3 (5%)
4	PGT	C	1566	-	50,50,50	0.93	2 (4%)	53,56,56	1.05	4 (7%)
2	FLC	C	1569	-	12,12,12	1.14	0	17,17,17	1.12	1 (5%)
4	PGT	A	1590	-	50,50,50	0.95	2 (4%)	53,56,56	1.05	4 (7%)

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
4	PGT	A	1591	-	-	6/15/15/55	-
2	FLC	C	1001	-	-	4/16/16/16	-
5	PEG	B	1555	-	-	0/4/4/4	-
4	PGT	A	1592	-	-	26/55/55/55	-
4	PGT	C	1565	-	-	16/55/55/55	-
4	PGT	B	1554	-	-	16/55/55/55	-
2	FLC	B	1001	-	-	6/16/16/16	-
4	PGT	C	1567	-	-	21/55/55/55	-
2	FLC	A	1001	-	-	4/16/16/16	-
6	CM5	C	1568	-	-	6/17/65/65	0/3/3/3
4	PGT	A	1589	-	-	20/55/55/55	-
4	PGT	A	1588	-	-	21/55/55/55	-
4	PGT	C	1566	-	-	18/55/55/55	-
2	FLC	C	1569	-	-	7/16/16/16	-
4	PGT	A	1590	-	-	31/55/55/55	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1589	PGT	O3-C11	4.53	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1590	PGT	O3-C11	4.46	1.46	1.33
4	A	1592	PGT	O3-C11	4.34	1.46	1.33
4	A	1589	PGT	O2-C31	4.33	1.46	1.34
4	C	1567	PGT	O3-C11	4.32	1.45	1.33
4	A	1588	PGT	O2-C31	4.28	1.46	1.34
4	C	1565	PGT	O3-C11	4.28	1.45	1.33
4	C	1566	PGT	O3-C11	4.25	1.45	1.33
4	B	1554	PGT	O3-C11	4.25	1.45	1.33
4	A	1588	PGT	O3-C11	4.23	1.45	1.33
4	B	1554	PGT	O2-C31	4.23	1.46	1.34
4	C	1567	PGT	O2-C31	4.19	1.46	1.34
4	C	1566	PGT	O2-C31	4.13	1.45	1.34
4	A	1592	PGT	O2-C31	4.06	1.45	1.34
4	C	1565	PGT	O2-C31	4.04	1.45	1.34
4	A	1590	PGT	O2-C31	4.01	1.45	1.34
2	B	1001	FLC	CB-CBC	-2.42	1.50	1.53
2	C	1001	FLC	CB-CBC	-2.37	1.51	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1588	PGT	O2-C31-C32	4.61	121.46	111.48
4	C	1566	PGT	O2-C31-C32	4.28	120.74	111.48
4	B	1554	PGT	O2-C31-C32	4.08	120.31	111.48
4	A	1592	PGT	O2-C31-C32	3.93	119.98	111.48
4	C	1567	PGT	O2-C31-C32	3.85	119.82	111.48
4	A	1589	PGT	O2-C31-C32	3.78	119.65	111.48
4	A	1590	PGT	O2-C31-C32	3.62	119.32	111.48
4	A	1590	PGT	C2-O2-C31	-3.57	109.26	117.80
4	C	1565	PGT	C2-O2-C31	-3.53	109.35	117.80
4	C	1565	PGT	O2-C31-C32	3.50	119.06	111.48
6	C	1568	CM5	C24-O23-C16	-2.98	110.92	117.98
2	A	1001	FLC	OB2-CBC-CB	2.93	118.76	113.14
4	A	1589	PGT	O3-C11-C12	2.92	120.75	111.83
4	A	1590	PGT	O3-C11-C12	2.87	120.58	111.83
2	B	1001	FLC	OB2-CBC-CB	2.84	118.59	113.14
2	C	1569	FLC	OB2-CBC-CB	2.82	118.55	113.14
4	A	1592	PGT	O3-C11-C12	2.77	120.29	111.83
4	A	1588	PGT	O3-C11-C12	2.74	120.20	111.83
2	C	1001	FLC	OB2-CBC-CB	2.73	118.38	113.14
4	C	1567	PGT	O3-C11-C12	2.68	120.00	111.83
4	C	1566	PGT	C2-O2-C31	-2.63	111.50	117.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1554	PGT	O3-C11-C12	2.52	119.52	111.83
4	C	1566	PGT	O3-C11-C12	2.38	119.11	111.83
4	A	1588	PGT	O2-C31-O31	-2.29	118.36	123.70
4	C	1565	PGT	O3-C11-C12	2.24	118.68	111.83
4	C	1567	PGT	C2-O2-C31	-2.13	112.71	117.80
4	C	1566	PGT	O2-C31-O31	-2.05	118.90	123.70
4	B	1554	PGT	C2-O2-C31	-2.04	112.92	117.80
4	A	1590	PGT	O2-C31-O31	-2.04	118.94	123.70
4	A	1592	PGT	O2-C31-O31	-2.03	118.97	123.70

There are no chirality outliers.

All (202) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	FLC	CA-CB-CBC-OB1
2	A	1001	FLC	CA-CB-CBC-OB2
2	A	1001	FLC	OHB-CB-CBC-OB1
2	A	1001	FLC	OHB-CB-CBC-OB2
2	B	1001	FLC	CA-CB-CBC-OB1
2	B	1001	FLC	CA-CB-CBC-OB2
2	B	1001	FLC	OHB-CB-CBC-OB1
2	B	1001	FLC	OHB-CB-CBC-OB2
2	C	1001	FLC	CA-CB-CBC-OB1
2	C	1001	FLC	CA-CB-CBC-OB2
2	C	1001	FLC	OHB-CB-CBC-OB1
2	C	1001	FLC	OHB-CB-CBC-OB2
2	C	1569	FLC	CA-CB-CBC-OB1
2	C	1569	FLC	CA-CB-CBC-OB2
2	C	1569	FLC	OHB-CB-CBC-OB1
2	C	1569	FLC	OHB-CB-CBC-OB2
2	C	1569	FLC	CA-CB-CG-CGC
2	C	1569	FLC	OHB-CB-CG-CGC
4	A	1588	PGT	O31-C31-O2-C2
4	A	1588	PGT	C1-O3P-P-O2P
4	A	1588	PGT	C1-O3P-P-O4P
4	A	1589	PGT	C1-O3P-P-O2P
4	A	1589	PGT	C1-O3P-P-O4P
4	A	1589	PGT	C4-O4P-P-O1P
4	A	1590	PGT	C4-O4P-P-O3P
4	A	1590	PGT	C4-O4P-P-O1P
4	A	1590	PGT	C4-O4P-P-O2P
4	A	1590	PGT	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1590	PGT	O5-C5-C6-O6
4	A	1592	PGT	C32-C31-O2-C2
4	A	1592	PGT	C1-O3P-P-O1P
4	A	1592	PGT	C1-O3P-P-O2P
4	A	1592	PGT	C1-O3P-P-O4P
4	A	1592	PGT	C4-O4P-P-O3P
4	A	1592	PGT	C4-O4P-P-O1P
4	A	1592	PGT	C4-O4P-P-O2P
4	B	1554	PGT	C1-O3P-P-O2P
4	B	1554	PGT	C1-O3P-P-O4P
4	C	1565	PGT	C32-C31-O2-C2
4	C	1565	PGT	O31-C31-O2-C2
4	C	1565	PGT	C1-O3P-P-O1P
4	C	1565	PGT	C1-O3P-P-O2P
4	C	1566	PGT	C32-C31-O2-C2
4	C	1566	PGT	O31-C31-O2-C2
4	C	1566	PGT	C1-O3P-P-O2P
4	C	1566	PGT	C1-O3P-P-O4P
4	C	1567	PGT	C32-C31-O2-C2
4	C	1567	PGT	C1-O3P-P-O4P
6	C	1568	CM5	O14-C13-O12-C1
4	A	1590	PGT	O31-C31-O2-C2
4	C	1567	PGT	O31-C31-O2-C2
4	A	1588	PGT	C32-C31-O2-C2
4	A	1590	PGT	C32-C31-O2-C2
4	A	1590	PGT	C12-C11-O3-C3
4	A	1592	PGT	O31-C31-O2-C2
4	C	1566	PGT	O4P-C4-C5-O5
4	A	1589	PGT	C12-C11-O3-C3
4	A	1590	PGT	O11-C11-O3-C3
4	A	1589	PGT	O11-C11-O3-C3
4	A	1588	PGT	C12-C11-O3-C3
4	C	1567	PGT	C37-C38-C39-C40
4	C	1567	PGT	C11-C12-C13-C14
4	A	1591	PGT	C37-C38-C39-C40
4	A	1590	PGT	C31-C32-C33-C34
4	A	1592	PGT	C19-C20-C21-C22
4	A	1588	PGT	O11-C11-O3-C3
4	A	1588	PGT	C11-C12-C13-C14
2	C	1569	FLC	CBC-CB-CG-CGC
6	C	1568	CM5	C18-C13-O12-C1
6	C	1568	CM5	O12-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	1590	PGT	C2-C1-O3P-P
4	B	1554	PGT	C42-C43-C44-C45
4	A	1590	PGT	C22-C23-C24-C25
4	A	1592	PGT	C15-C16-C17-C18
4	A	1591	PGT	C38-C39-C40-C41
4	C	1566	PGT	C18-C19-C20-C21
4	A	1590	PGT	C44-C45-C46-C47
4	A	1590	PGT	C12-C13-C14-C15
4	C	1567	PGT	C12-C13-C14-C15
6	C	1568	CM5	O25-C26-C30-O31
4	A	1589	PGT	C32-C31-O2-C2
4	B	1554	PGT	C41-C42-C43-C44
4	A	1588	PGT	C20-C21-C22-C23
4	C	1565	PGT	C44-C45-C46-C47
4	A	1591	PGT	C40-C41-C42-C43
4	C	1565	PGT	C13-C14-C15-C16
4	A	1590	PGT	C41-C42-C43-C44
4	A	1588	PGT	C40-C41-C42-C43
4	B	1554	PGT	C12-C11-O3-C3
4	A	1592	PGT	C23-C24-C25-C26
4	A	1589	PGT	C22-C23-C24-C25
4	A	1589	PGT	O31-C31-O2-C2
4	C	1567	PGT	C17-C18-C19-C20
4	A	1589	PGT	C33-C34-C35-C36
4	A	1590	PGT	C2-C3-O3-C11
4	B	1554	PGT	O11-C11-O3-C3
4	A	1589	PGT	C44-C45-C46-C47
4	A	1590	PGT	C11-C12-C13-C14
4	A	1588	PGT	O3P-C1-C2-O2
4	A	1590	PGT	C14-C15-C16-C17
4	C	1566	PGT	C44-C45-C46-C47
4	A	1588	PGT	C23-C24-C25-C26
4	C	1567	PGT	C13-C14-C15-C16
4	B	1554	PGT	C40-C41-C42-C43
4	C	1566	PGT	C33-C34-C35-C36
4	C	1567	PGT	C41-C42-C43-C44
4	A	1591	PGT	C36-C37-C38-C39
4	C	1566	PGT	O4P-C4-C5-C6
4	B	1554	PGT	C1-C2-C3-O3
4	C	1565	PGT	C1-C2-C3-O3
4	A	1589	PGT	O3P-C1-C2-O2
4	C	1566	PGT	O3P-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	1589	PGT	C34-C35-C36-C37
4	A	1592	PGT	C12-C13-C14-C15
4	B	1554	PGT	C34-C35-C36-C37
4	A	1589	PGT	O3P-C1-C2-C3
4	A	1592	PGT	O3P-C1-C2-C3
4	C	1566	PGT	O3P-C1-C2-C3
4	C	1567	PGT	C34-C35-C36-C37
4	C	1567	PGT	C21-C22-C23-C24
4	A	1592	PGT	C17-C18-C19-C20
4	A	1588	PGT	C1-C2-O2-C31
4	A	1590	PGT	C45-C46-C47-C48
4	C	1565	PGT	C14-C15-C16-C17
4	A	1592	PGT	O3P-C1-C2-O2
4	A	1589	PGT	C1-C2-C3-O3
4	A	1589	PGT	O2-C2-C3-O3
4	B	1554	PGT	O2-C2-C3-O3
4	C	1565	PGT	O2-C2-C3-O3
4	A	1590	PGT	C19-C20-C21-C22
4	A	1591	PGT	C33-C34-C35-C36
4	A	1590	PGT	C13-C14-C15-C16
4	A	1589	PGT	C43-C44-C45-C46
4	C	1567	PGT	C32-C33-C34-C35
4	C	1567	PGT	C20-C21-C22-C23
4	A	1589	PGT	C2-C1-O3P-P
4	A	1592	PGT	C2-C1-O3P-P
4	A	1592	PGT	C13-C14-C15-C16
4	A	1590	PGT	C32-C33-C34-C35
4	C	1567	PGT	C43-C44-C45-C46
6	C	1568	CM5	C2-C3-C4-C5
2	B	1001	FLC	CBC-CB-CG-CGC
4	A	1588	PGT	C4-O4P-P-O1P
4	C	1565	PGT	C1-O3P-P-O4P
4	C	1566	PGT	C1-O3P-P-O1P
4	C	1565	PGT	C40-C41-C42-C43
4	A	1588	PGT	C2-C1-O3P-P
4	A	1590	PGT	C5-C4-O4P-P
4	C	1567	PGT	C2-C1-O3P-P
4	A	1592	PGT	C1-C2-O2-C31
4	C	1566	PGT	C3-C2-O2-C31
4	B	1554	PGT	C18-C19-C20-C21
4	A	1588	PGT	O3P-C1-C2-C3
4	B	1554	PGT	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
4	B	1554	PGT	C19-C20-C21-C22
2	B	1001	FLC	OHB-CB-CG-CGC
4	A	1592	PGT	O2-C2-C3-O3
4	A	1590	PGT	C17-C18-C19-C20
4	A	1588	PGT	C21-C22-C23-C24
4	C	1566	PGT	C12-C11-O3-C3
4	A	1590	PGT	C39-C40-C41-C42
4	A	1590	PGT	C42-C43-C44-C45
4	C	1566	PGT	O11-C11-O3-C3
4	A	1592	PGT	C18-C19-C20-C21
4	C	1565	PGT	C39-C40-C41-C42
4	C	1566	PGT	C1-C2-O2-C31
4	C	1567	PGT	C40-C41-C42-C43
4	A	1588	PGT	C38-C39-C40-C41
4	A	1592	PGT	C32-C33-C34-C35
4	C	1565	PGT	C42-C43-C44-C45
4	B	1554	PGT	C33-C34-C35-C36
4	C	1567	PGT	O3-C11-C12-C13
4	A	1590	PGT	C40-C41-C42-C43
4	C	1567	PGT	C5-C4-O4P-P
4	A	1592	PGT	O4P-C4-C5-C6
4	A	1588	PGT	C41-C42-C43-C44
4	A	1588	PGT	C44-C45-C46-C47
4	A	1591	PGT	C44-C45-C46-C47
4	C	1567	PGT	O2-C31-C32-C33
4	A	1592	PGT	C41-C42-C43-C44
4	A	1588	PGT	O2-C31-C32-C33
4	A	1590	PGT	C37-C38-C39-C40
4	A	1589	PGT	O2-C31-C32-C33
4	C	1566	PGT	C39-C40-C41-C42
4	A	1589	PGT	C23-C24-C25-C26
4	C	1567	PGT	C31-C32-C33-C34
4	A	1590	PGT	O2-C31-C32-C33
4	A	1592	PGT	O2-C31-C32-C33
4	C	1565	PGT	C18-C19-C20-C21
4	A	1590	PGT	C36-C37-C38-C39
4	B	1554	PGT	C45-C46-C47-C48
4	C	1565	PGT	C32-C33-C34-C35
4	C	1567	PGT	O3P-C1-C2-C3
4	A	1590	PGT	O31-C31-C32-C33
4	C	1566	PGT	C32-C33-C34-C35
4	B	1554	PGT	C21-C22-C23-C24

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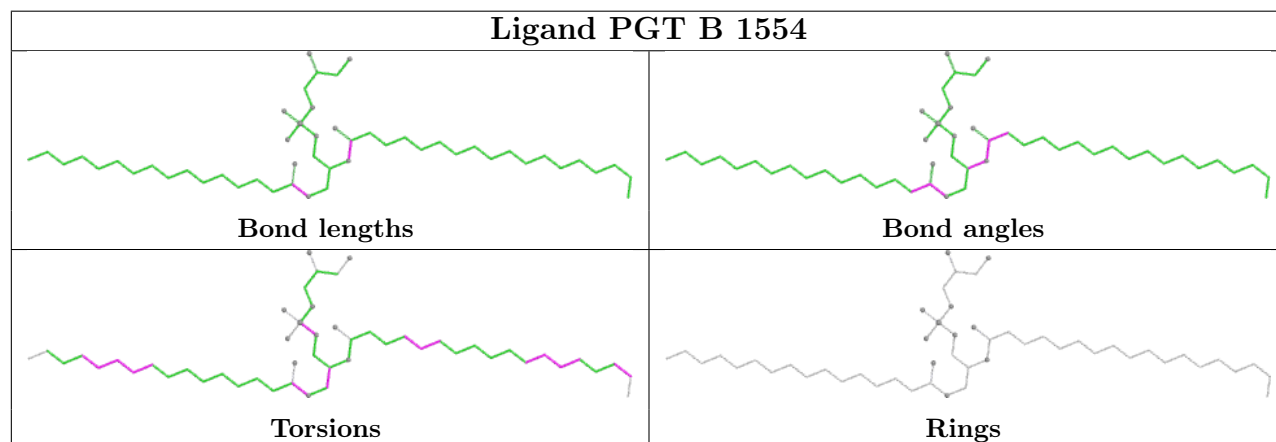
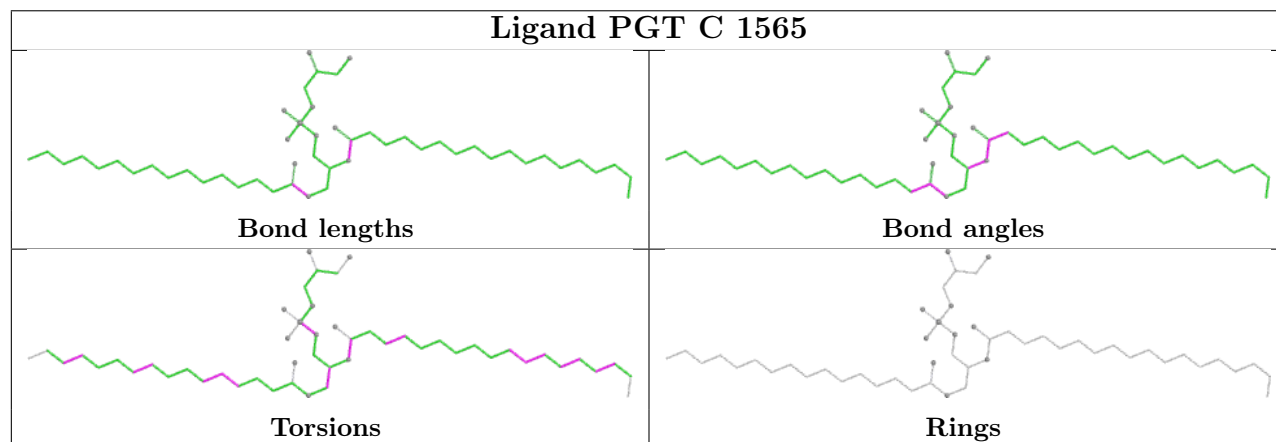
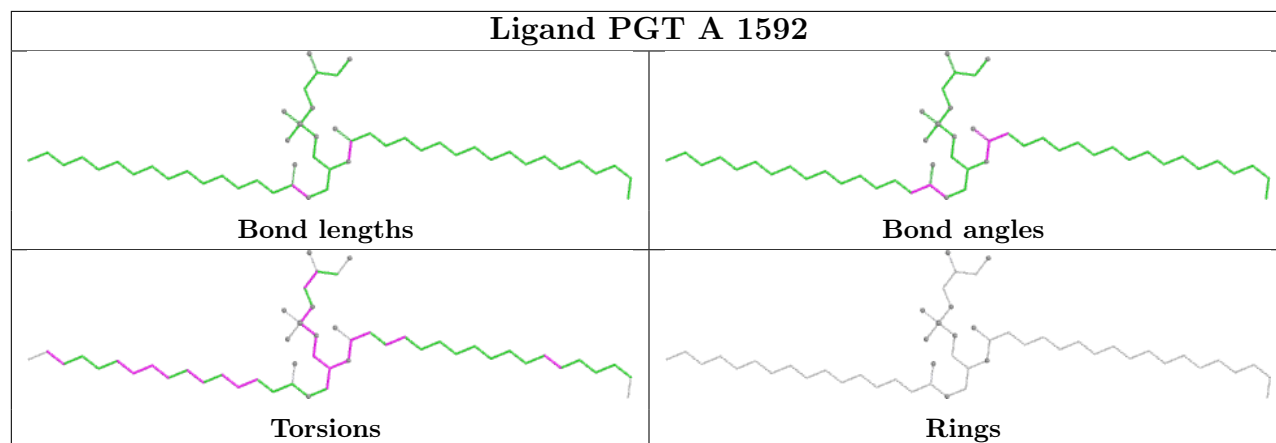
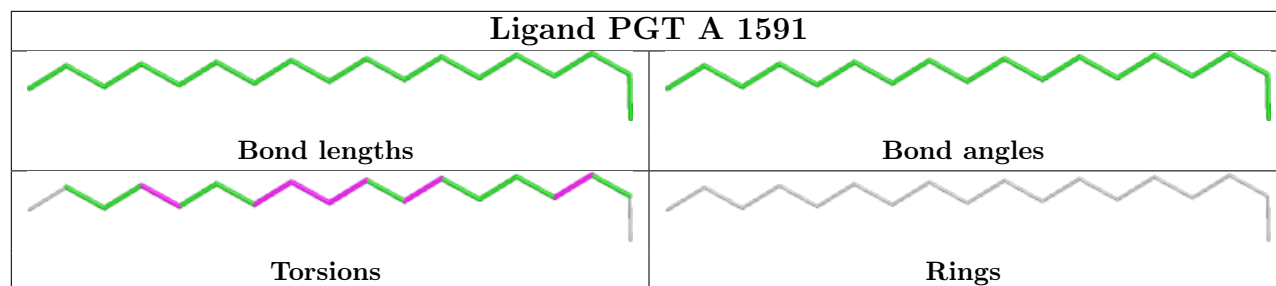
Mol	Chain	Res	Type	Atoms
4	A	1592	PGT	C1-C2-C3-O3
4	A	1588	PGT	O31-C31-C32-C33
4	A	1589	PGT	O31-C31-C32-C33
4	A	1592	PGT	O31-C31-C32-C33
6	C	1568	CM5	C1-C2-C3-C4
4	C	1565	PGT	C22-C23-C24-C25

There are no ring outliers.

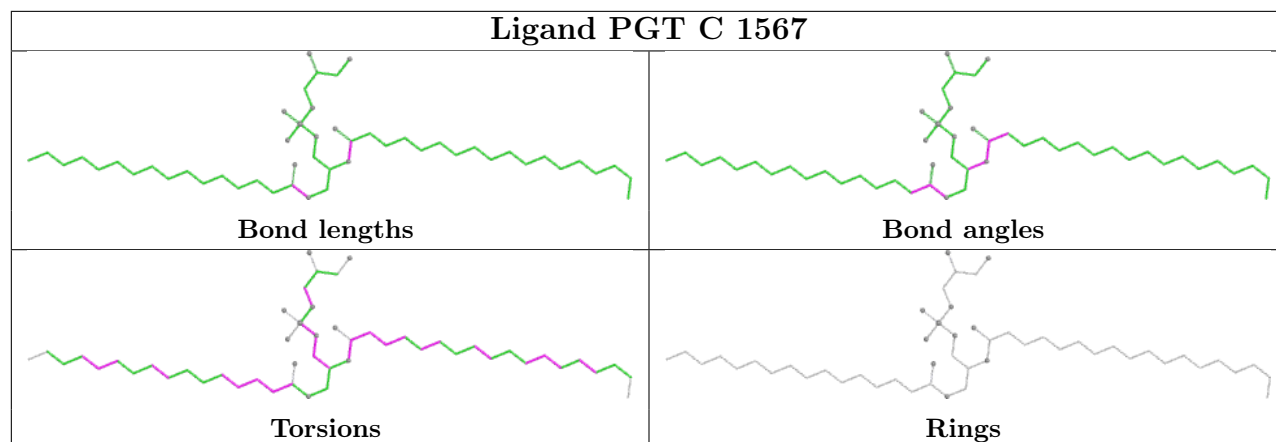
12 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1591	PGT	1	0
2	C	1001	FLC	2	0
4	A	1592	PGT	6	0
4	C	1565	PGT	8	0
4	B	1554	PGT	5	0
2	B	1001	FLC	3	0
4	C	1567	PGT	6	0
6	C	1568	CM5	3	0
4	A	1589	PGT	16	0
4	A	1588	PGT	8	0
4	C	1566	PGT	2	0
4	A	1590	PGT	4	0

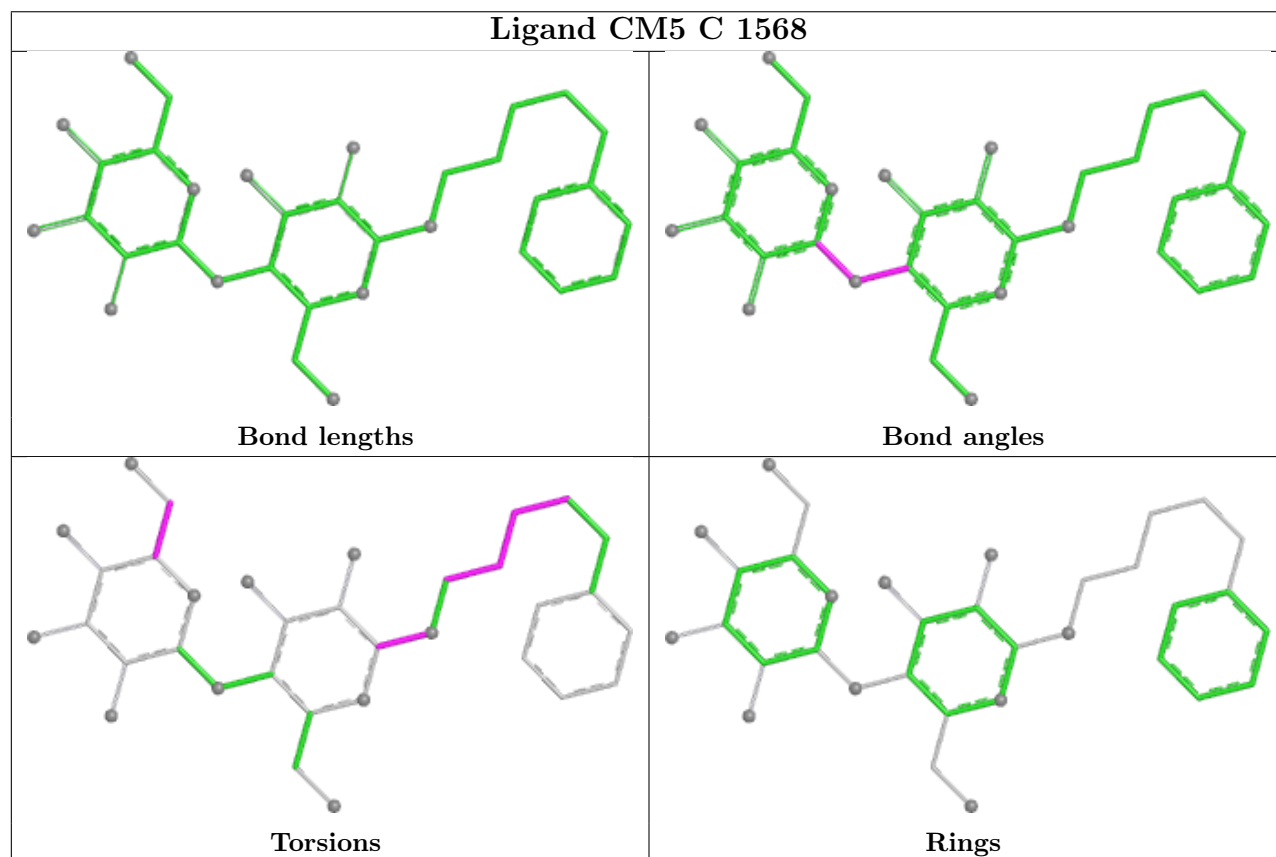
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



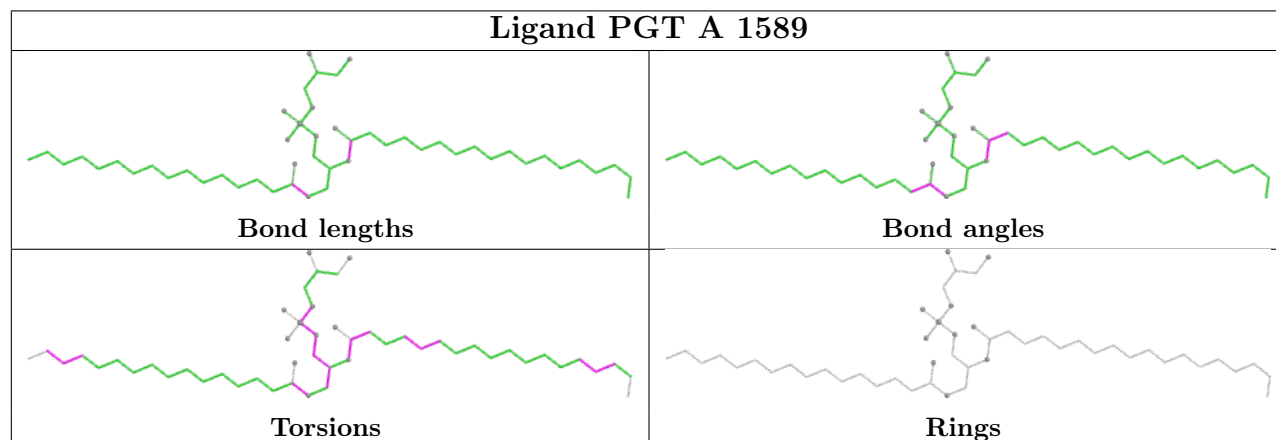
Ligand PGT C 1567

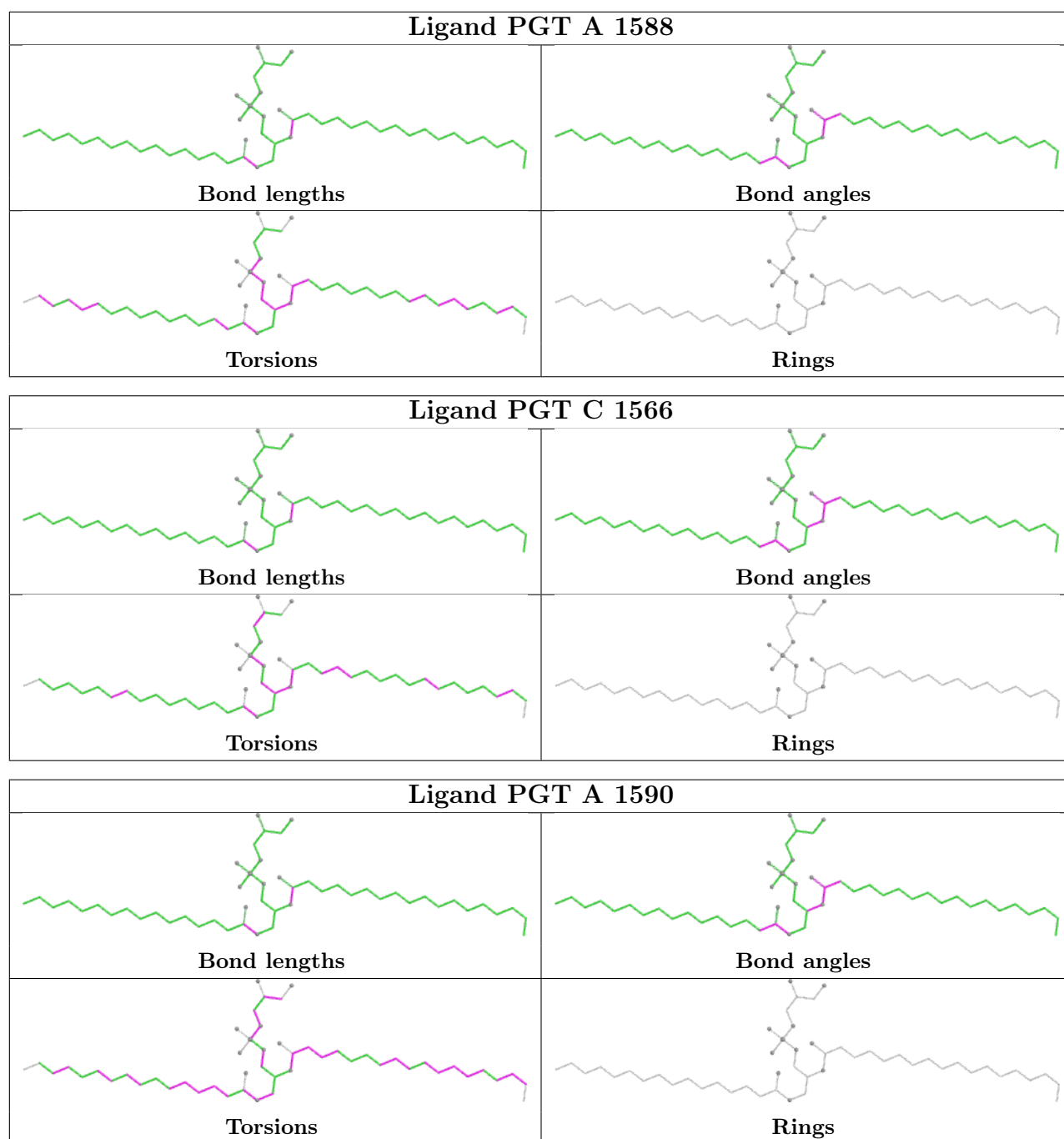


Ligand CM5 C 1568



Ligand PGT A 1589





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	531/566 (93%)	0.19	29 (5%)	30 27	58, 102, 170, 244	1 (0%)
1	B	497/566 (87%)	0.23	27 (5%)	31 27	48, 104, 176, 248	0
1	C	506/566 (89%)	0.03	13 (2%)	57 54	48, 86, 159, 215	0
All	All	1534/1698 (90%)	0.15	69 (4%)	38 34	48, 98, 170, 248	1 (0%)

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	550	TYR	6.2
1	C	561	ALA	4.8
1	B	485	LEU	4.4
1	B	549	ILE	4.0
1	A	150	MET	3.7
1	C	554	ARG	3.6
1	A	490	TRP	3.6
1	A	522	THR	3.6
1	B	432	GLY	3.4
1	A	277	TRP	3.3
1	C	277	TRP	3.3
1	C	276	ASP	3.3
1	A	403	LEU	3.2
1	A	475	VAL	3.2
1	A	278	THR	3.0
1	A	521	VAL	3.0
1	C	137	ARG	3.0
1	A	572	GLU	2.9
1	A	153	GLY	2.9
1	B	141	TRP	2.8
1	A	154	LEU	2.8
1	A	446	ALA	2.8
1	B	484	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	416	PHE	2.8
1	C	550	TYR	2.8
1	A	506	LEU	2.7
1	B	455	ILE	2.7
1	B	58	LEU	2.7
1	A	149	GLY	2.5
1	B	377	TRP	2.5
1	B	490	TRP	2.5
1	A	359	ALA	2.5
1	C	141	TRP	2.5
1	C	136	PHE	2.5
1	A	447	LEU	2.4
1	A	87	PHE	2.4
1	C	274	PRO	2.4
1	B	171	PRO	2.4
1	B	548	VAL	2.4
1	A	525	ALA	2.4
1	A	248	PHE	2.3
1	A	553	TYR	2.3
1	B	174	ASP	2.3
1	B	433	ASP	2.3
1	A	445	HIS	2.3
1	B	140	SER	2.3
1	B	302	ILE	2.3
1	A	552	GLU	2.2
1	B	214	LYS	2.2
1	A	302	ILE	2.2
1	A	573	HIS	2.2
1	A	472	ALA	2.2
1	A	269	ASN	2.2
1	A	273	ASP	2.2
1	B	399	LEU	2.2
1	B	512	ASP	2.2
1	C	553	TYR	2.2
1	B	427	GLY	2.2
1	B	488	ASN	2.1
1	A	453	MET	2.1
1	B	129	ARG	2.1
1	B	479	MET	2.1
1	C	269	ASN	2.1
1	B	298	VAL	2.0
1	A	300	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	487	ALA	2.0
1	B	71	LEU	2.0
1	C	417	GLY	2.0
1	B	304	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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.

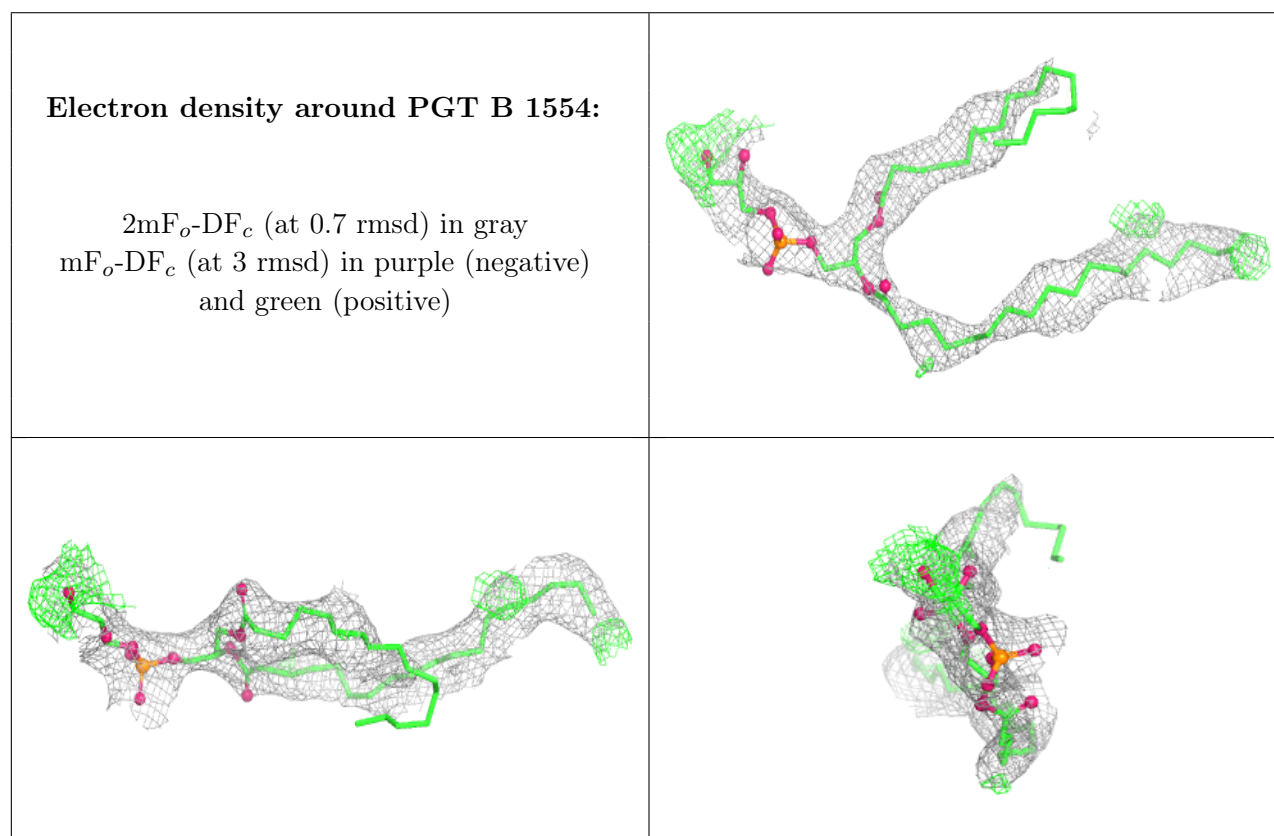
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PEG	B	1555	7/7	0.67	0.28	146,152,153,155	0
4	PGT	B	1554	51/51	0.72	0.21	72,136,208,240	0
2	FLC	C	1569	13/13	0.72	0.11	188,193,208,210	0
4	PGT	C	1567	51/51	0.76	0.18	107,157,233,319	0
4	PGT	C	1566	51/51	0.78	0.21	109,144,184,223	0
4	PGT	C	1565	51/51	0.79	0.19	106,176,230,291	0
4	PGT	A	1588	51/51	0.79	0.17	85,136,175,236	0
4	PGT	A	1592	51/51	0.80	0.18	69,150,203,314	0
4	PGT	A	1589	51/51	0.80	0.21	74,132,232,385	0
3	CL	A	1587	1/1	0.82	0.18	105,105,105,105	0
4	PGT	A	1590	51/51	0.83	0.20	72,99,130,231	0
2	FLC	B	1001	13/13	0.84	0.27	140,150,161,162	0
6	CM5	C	1568	34/34	0.87	0.12	112,182,209,211	0
4	PGT	A	1591	18/51	0.88	0.17	86,92,114,114	0
3	CL	C	1564	1/1	0.91	0.13	85,85,85,85	0
2	FLC	A	1001	13/13	0.91	0.19	147,163,169,170	0
2	FLC	C	1001	13/13	0.93	0.16	133,140,145,145	0
3	CL	B	1553	1/1	0.94	0.13	109,109,109,109	0
3	CL	C	1563	1/1	0.97	0.07	64,64,64,64	0

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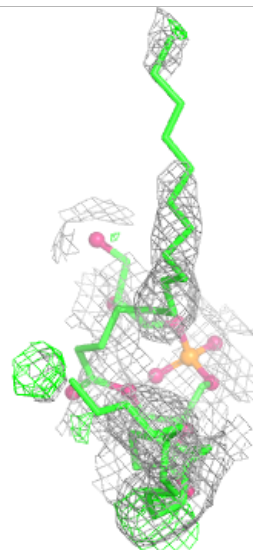
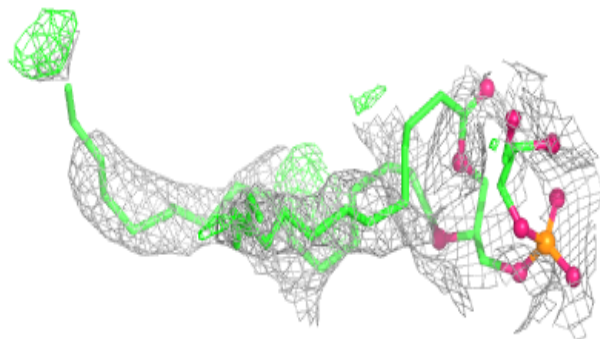
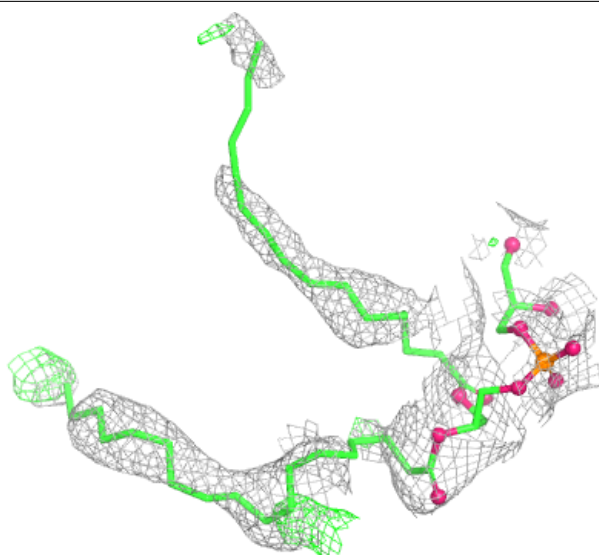
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	C	1562	1/1	0.98	0.14	74,74,74,74	0

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.



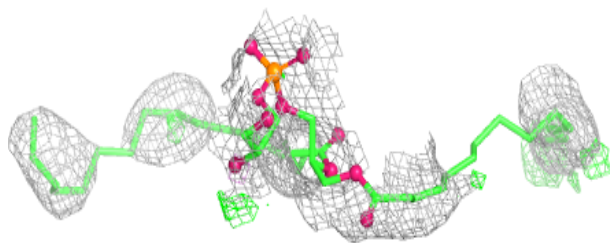
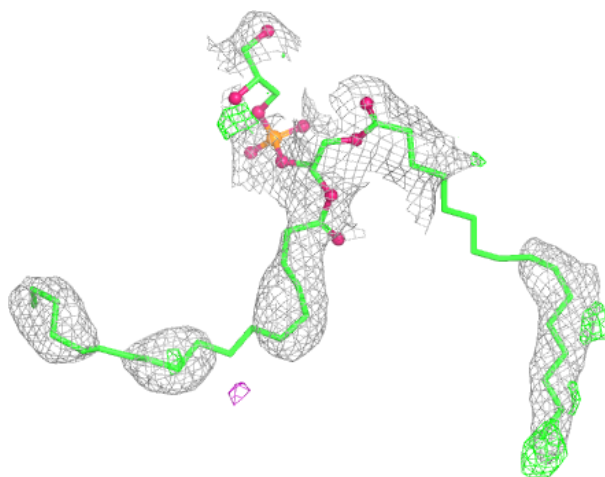
Electron density around PGT C 1567:

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



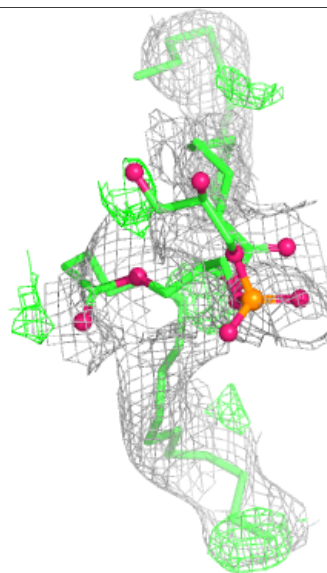
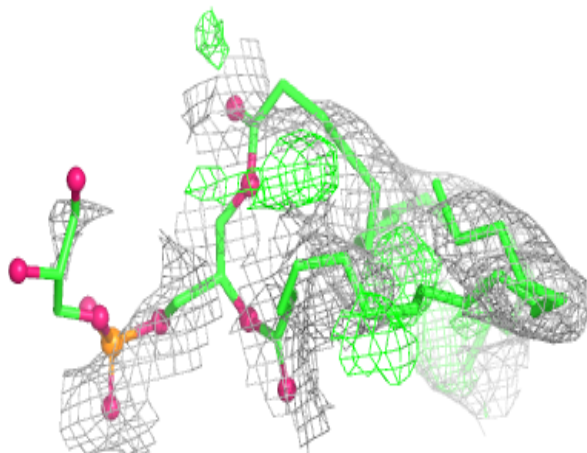
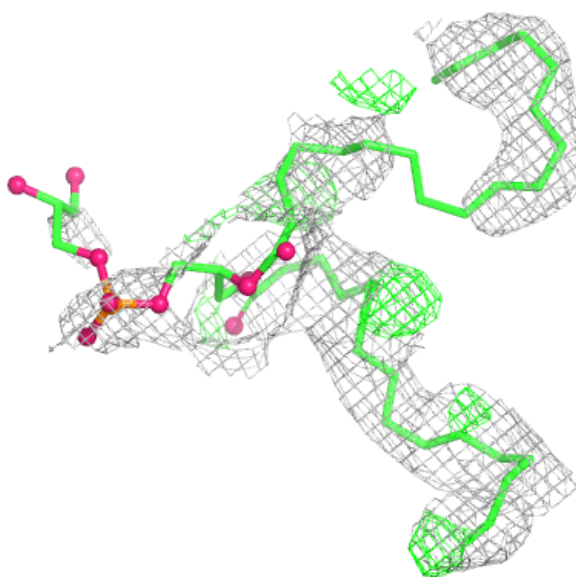
Electron density around PGT C 1566:

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



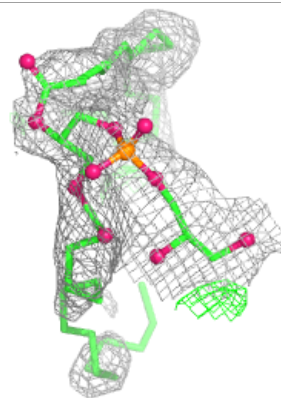
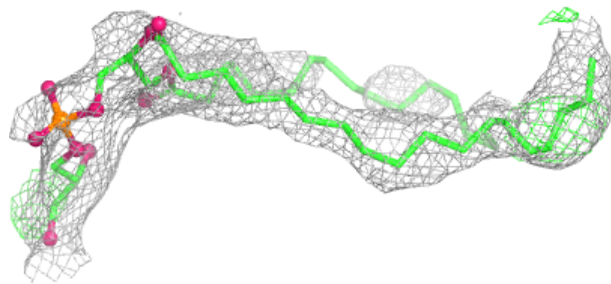
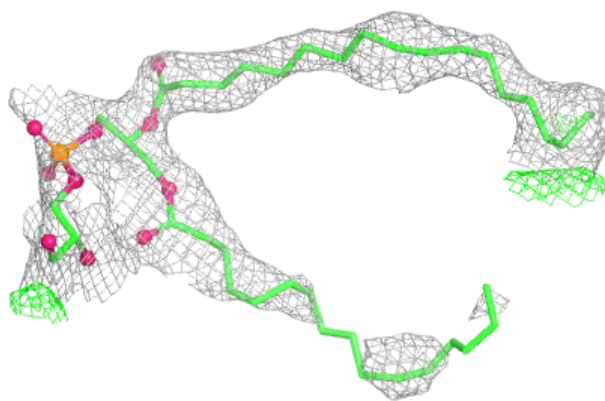
Electron density around PGT C 1565:

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



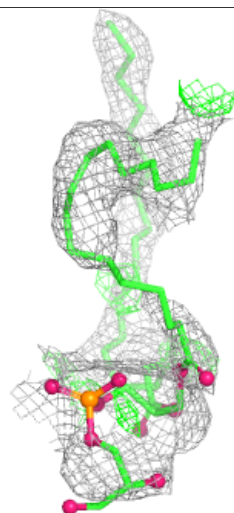
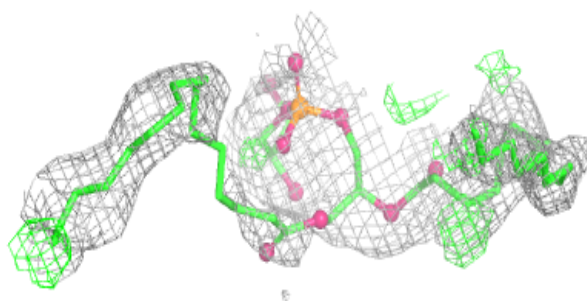
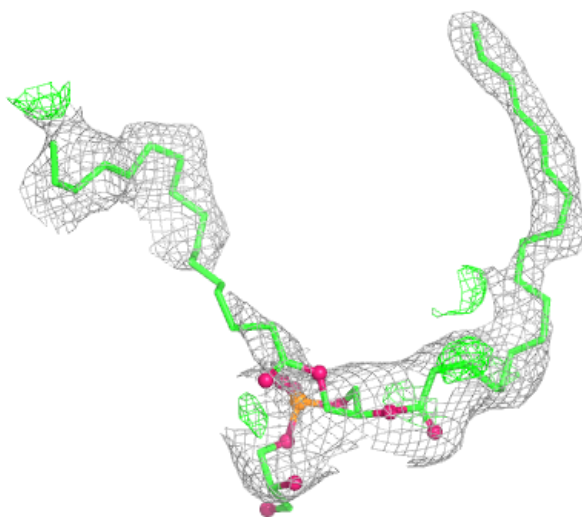
Electron density around PGT A 1588:

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



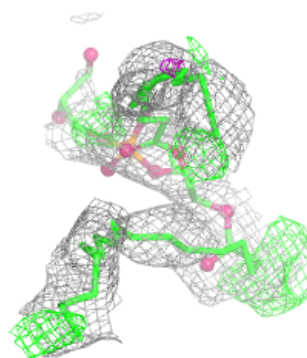
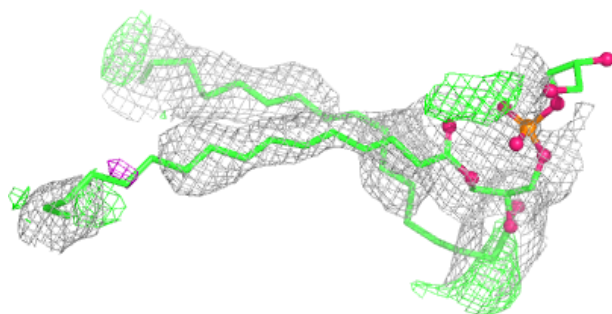
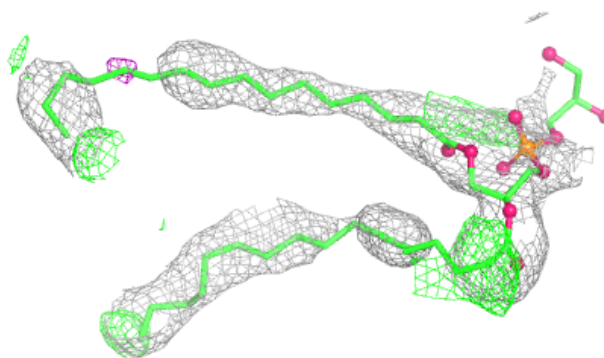
Electron density around PGT A 1592:

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

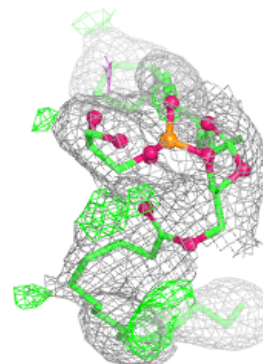
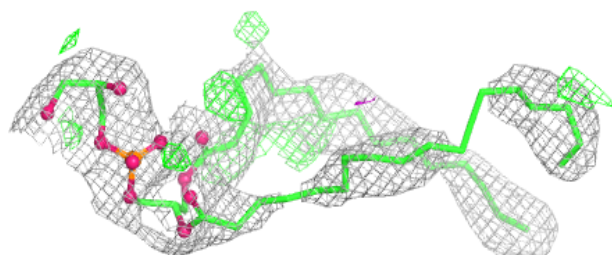
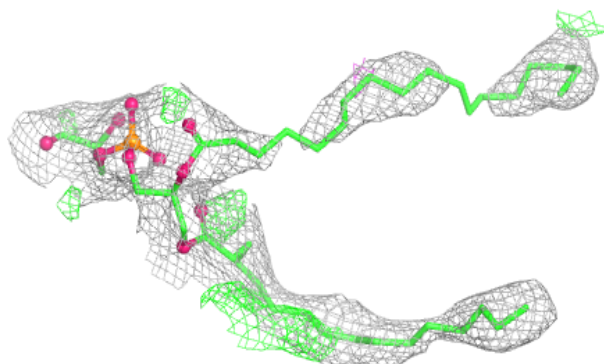


Electron density around PGT A 1589:

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

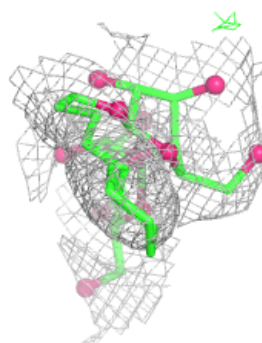
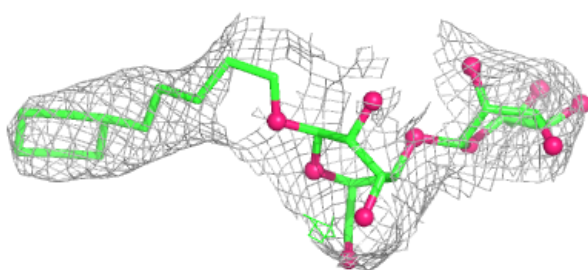
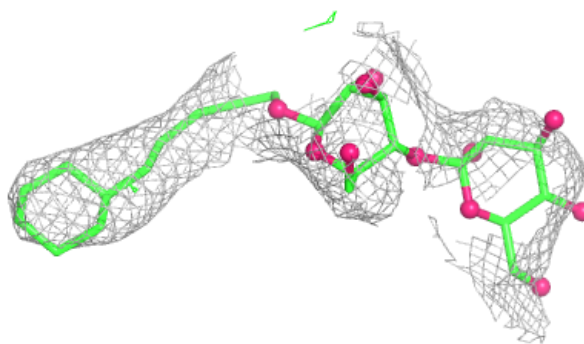
**Electron density around PGT A 1590:**

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

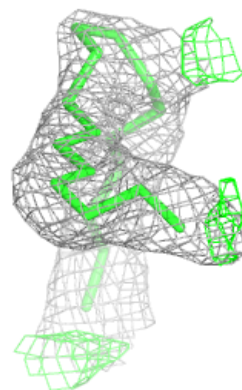
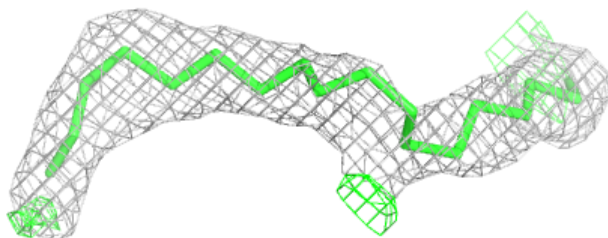
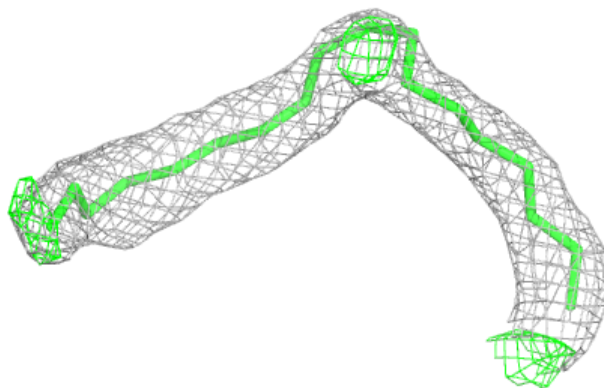


Electron density around CM5 C 1568:

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

**Electron density around PGT A 1591:**

$2mF_o-DF_c$ (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.