



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:37 AM UTC

PDB ID : 2ZVT / pdb_00002zvt
Title : Cys285Ser mutant PPARgamma ligand-binding domain complexed with 15-d
eoxy-delta12,14-prostaglandin J2
Authors : Waku, T.; Oyama, T.; Shiraki, T.; Morikawa, K.
Deposited on : 2008-11-19
Resolution : 1.90 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

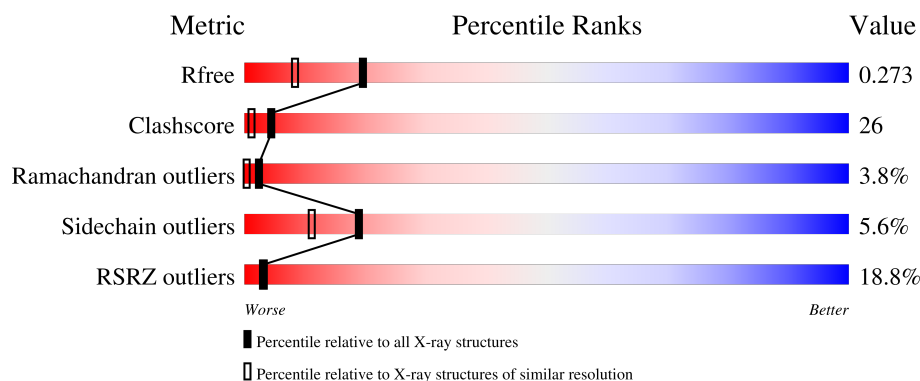
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	286	19% 62% 27% 7% • •
1	B	286	16% 55% 29% 6% • 8%

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	PTG	B	2	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4538 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

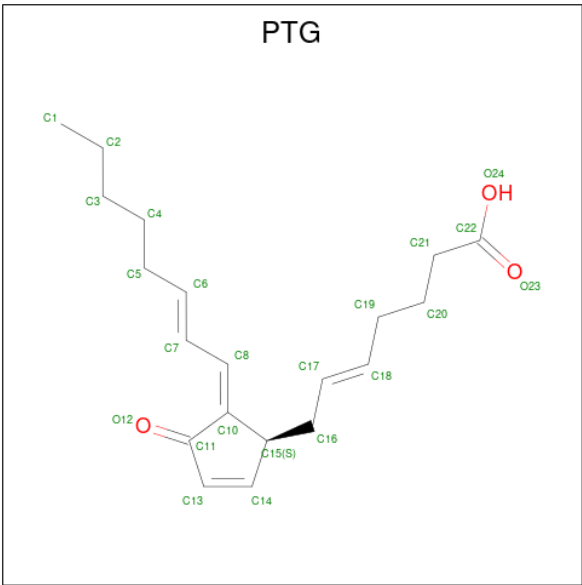
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2198	1417	360	412	9			
1	B	263	Total	C	N	O	S	0	0	0
			2110	1363	346	393	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	MET	-	expression tag	UNP P37231
A	285	SER	CYS	engineered mutation	UNP P37231
B	191	GLY	-	expression tag	UNP P37231
B	192	SER	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	UNP P37231
B	194	MET	-	expression tag	UNP P37231
B	285	SER	CYS	engineered mutation	UNP P37231

- Molecule 2 is (5E,14E)-11-oxoprostano-5,9,12,14-tetraen-1-oic acid (CCD ID: PTG) (formula: $C_{20}H_{28}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	20	3		
2	B	1	Total	C	O	0	0
			23	20	3		

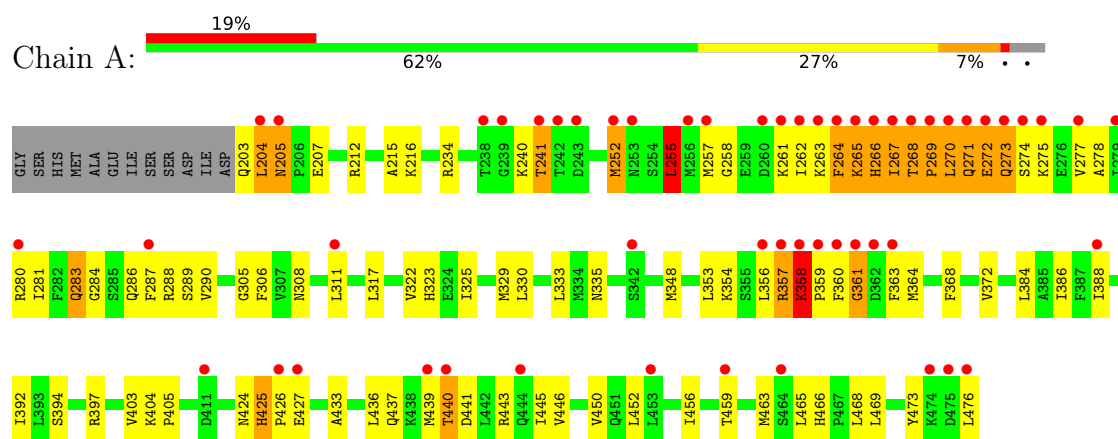
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	92	Total	O	0	0
			92	92		
3	B	92	Total	O	0	0
			92	92		

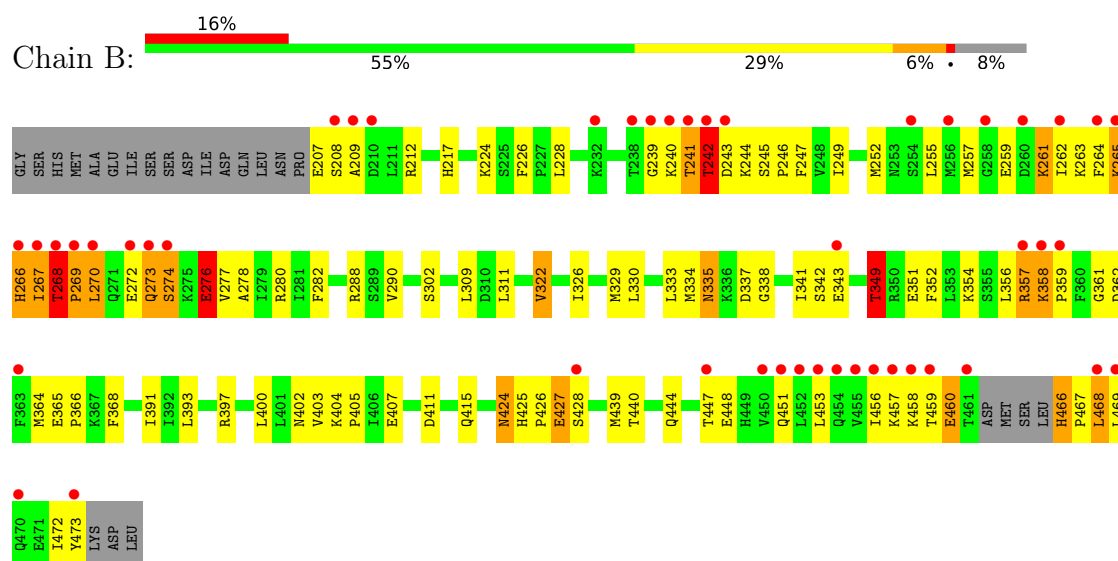
3 Residue-property plots

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: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.98Å 61.39Å 118.54Å 90.00° 102.89° 90.00°	Depositor
Resolution (Å)	29.67 – 1.90 29.67 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.67-1.90) 94.0 (29.67-1.90)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.275 0.249 , 0.273	Depositor DCC
R_{free} test set	2364 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4538	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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: PTG

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	0.44	0/2236	0.98	13/3013 (0.4%)
1	B	0.42	0/2146	1.00	10/2891 (0.3%)
All	All	0.43	0/4382	0.99	23/5904 (0.4%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	267	ILE	N-CA-C	-11.14	86.16	109.34
1	B	266	HIS	N-CA-C	9.57	127.86	107.67
1	A	205	ASN	N-CA-C	8.22	123.19	109.87
1	B	466	HIS	CA-C-N	8.00	129.84	119.84
1	B	466	HIS	C-N-CA	8.00	129.84	119.84
1	A	241	THR	N-CA-C	7.57	119.72	110.41
1	B	268	THR	CA-C-N	7.39	129.07	119.84
1	B	268	THR	C-N-CA	7.39	129.07	119.84
1	A	335	ASN	N-CA-C	-7.25	98.29	109.24
1	A	267	ILE	N-CA-C	-7.06	103.47	113.07
1	A	205	ASN	CA-C-N	6.99	126.97	119.28
1	A	205	ASN	C-N-CA	6.99	126.97	119.28
1	B	322	VAL	N-CA-C	6.25	116.99	110.62
1	A	322	VAL	N-CA-C	5.93	116.67	110.62
1	A	255	LEU	N-CA-C	-5.83	105.01	111.36
1	B	349	THR	N-CA-C	5.45	118.13	110.23
1	A	306	PHE	N-CA-C	5.20	116.63	111.07
1	B	268	THR	N-CA-C	5.19	121.29	109.81
1	A	403	VAL	N-CA-C	5.15	117.53	111.09
1	B	242	THR	N-CA-C	-5.14	102.99	110.24
1	A	425	HIS	CA-C-N	5.14	125.18	119.32
1	A	425	HIS	C-N-CA	5.14	125.18	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	LEU	N-CA-C	5.11	121.68	110.80

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	2198	0	2264	95	0
1	B	2110	0	2174	141	0
2	A	23	0	27	2	0
2	B	23	0	27	10	0
3	A	92	0	0	1	0
3	B	92	0	0	6	0
All	All	4538	0	4492	234	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 (234) 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:B:349:THR:HG22	1:B:352:PHE:H	1.13	1.13
1:B:266:HIS:ND1	1:B:268:THR:HB	1.65	1.12
1:A:240:LYS:HG3	1:A:241:THR:HG23	1.35	1.05
1:A:358:LYS:HD2	1:A:358:LYS:H	1.28	0.98
1:B:459:THR:HG22	1:B:460:GLU:H	1.30	0.96
1:B:427:GLU:H	1:B:427:GLU:CD	1.73	0.96
1:A:205:ASN:HD22	1:A:207:GLU:HB2	1.29	0.95
1:B:358:LYS:HB3	1:B:359:PRO:CD	1.95	0.94
1:B:278:ALA:HB3	1:B:357:ARG:NH1	1.85	0.91
1:A:205:ASN:ND2	1:A:207:GLU:HB2	1.86	0.90
1:A:273:GLN:C	1:A:275:LYS:H	1.76	0.89
1:B:266:HIS:C	1:B:268:THR:H	1.77	0.89
1:A:272:GLU:HG2	1:A:273:GLN:H	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:HG2	1:A:273:GLN:HG3	1.59	0.85
1:B:335:ASN:C	1:B:335:ASN:HD22	1.85	0.85
1:B:326:ILE:HG23	2:B:2:PTG:H3	1.60	0.83
1:A:252:MET:HE3	1:A:252:MET:HA	1.61	0.81
1:B:268:THR:OG1	1:B:270:LEU:HG	1.84	0.78
1:B:335:ASN:ND2	1:B:337:ASP:H	1.82	0.78
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.66	0.77
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.66	0.77
1:A:240:LYS:HG3	1:A:241:THR:H	1.49	0.76
1:B:266:HIS:HB3	1:B:268:THR:HG22	1.65	0.76
1:B:266:HIS:C	1:B:268:THR:N	2.43	0.76
1:A:267:ILE:O	1:A:287:PHE:HB2	1.86	0.76
1:A:358:LYS:HD2	1:A:358:LYS:N	2.02	0.74
1:B:311:LEU:H	1:B:311:LEU:HD22	1.51	0.74
1:B:242:THR:O	1:B:244:LYS:N	2.21	0.74
1:B:264:PHE:O	1:B:265:LYS:C	2.31	0.73
1:B:349:THR:HG22	1:B:352:PHE:N	1.98	0.73
1:B:349:THR:CG2	1:B:352:PHE:H	1.98	0.71
1:B:391:ILE:HG12	1:B:439:MET:HE3	1.74	0.70
1:A:240:LYS:HG3	1:A:241:THR:CG2	2.19	0.69
1:B:459:THR:HG22	1:B:460:GLU:N	2.06	0.67
1:A:270:LEU:O	1:A:271:GLN:HG3	1.94	0.67
1:B:278:ALA:HB3	1:B:357:ARG:HH12	1.56	0.67
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.25	0.66
1:B:357:ARG:CZ	1:B:358:LYS:HD2	2.24	0.66
1:A:330:LEU:HD21	1:A:364:MET:HE1	1.78	0.66
1:B:244:LYS:O	1:B:244:LYS:HG3	1.96	0.66
1:B:425:HIS:HA	1:B:427:GLU:OE1	1.96	0.66
1:B:357:ARG:HH21	1:B:358:LYS:CE	2.09	0.65
1:B:357:ARG:NH2	1:B:358:LYS:HD2	2.10	0.65
1:B:311:LEU:HD22	1:B:311:LEU:N	2.11	0.65
1:A:273:GLN:C	1:A:275:LYS:N	2.47	0.65
1:B:208:SER:O	1:B:212:ARG:HG3	1.97	0.65
1:B:459:THR:CG2	1:B:460:GLU:H	2.03	0.64
1:A:273:GLN:O	1:A:275:LYS:N	2.31	0.63
1:B:358:LYS:HD3	1:B:460:GLU:OE1	1.98	0.63
1:B:252:MET:SD	1:B:277:VAL:HG21	2.38	0.63
1:B:261:LYS:HE3	1:B:261:LYS:HA	1.80	0.63
1:B:466:HIS:HD2	1:B:468:LEU:H	1.46	0.63
1:B:354:LYS:HA	1:B:361:GLY:O	1.99	0.63
1:A:270:LEU:HD23	1:A:270:LEU:C	2.22	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HG22	1:A:329:MET:HE2	1.81	0.62
1:B:447:THR:O	1:B:451:GLN:HG3	1.98	0.62
1:B:267:ILE:O	1:B:269:PRO:HD3	1.99	0.62
1:B:266:HIS:HB3	1:B:268:THR:CG2	2.29	0.62
1:B:357:ARG:HD3	1:B:357:ARG:C	2.24	0.62
1:A:441:ASP:O	1:A:445:ILE:HG12	2.00	0.61
1:A:452:LEU:O	1:A:456:ILE:HG12	2.01	0.61
1:B:335:ASN:HD22	1:B:337:ASP:H	1.50	0.60
1:A:252:MET:HE1	1:A:277:VAL:HG21	1.84	0.60
1:B:357:ARG:NH2	1:B:358:LYS:CE	2.65	0.59
1:A:288:ARG:HD2	1:A:288:ARG:O	2.01	0.59
1:B:278:ALA:CB	1:B:357:ARG:NH1	2.64	0.59
1:B:311:LEU:H	1:B:311:LEU:CD2	2.15	0.59
1:B:357:ARG:NH2	1:B:358:LYS:NZ	2.51	0.59
1:B:228:LEU:HD23	1:B:333:LEU:HD21	1.84	0.59
1:B:427:GLU:CD	1:B:427:GLU:N	2.53	0.59
1:A:240:LYS:HG3	1:A:241:THR:N	2.18	0.58
1:A:325:ILE:HG12	1:A:388:ILE:HG23	1.84	0.58
1:A:433:ALA:O	1:A:437:GLN:HG3	2.03	0.58
1:B:357:ARG:HH21	1:B:358:LYS:HE3	1.68	0.58
1:B:259:GLU:O	1:B:263:LYS:HA	2.04	0.57
1:B:330:LEU:HD13	2:B:2:PTG:H4	1.86	0.57
1:A:288:ARG:HG3	2:A:1:PTG:O12	2.04	0.57
1:A:212:ARG:O	1:A:216:LYS:HG2	2.04	0.56
1:A:368:PHE:O	1:A:372:VAL:HG23	2.05	0.56
1:B:252:MET:SD	1:B:277:VAL:HG11	2.46	0.56
1:B:335:ASN:ND2	1:B:338:GLY:H	2.03	0.56
1:B:269:PRO:O	1:B:270:LEU:C	2.48	0.56
1:A:272:GLU:CG	1:A:273:GLN:H	2.09	0.55
1:B:265:LYS:HG3	3:B:1090:HOH:O	2.06	0.55
1:A:323:HIS:CE1	1:A:473:TYR:OH	2.60	0.55
1:A:268:THR:CG2	1:A:280:ARG:HH11	2.18	0.55
1:B:266:HIS:O	1:B:268:THR:HG22	2.07	0.55
1:B:278:ALA:HB3	1:B:357:ARG:HH11	1.68	0.55
1:B:288:ARG:HG3	2:B:2:PTG:H2A	1.89	0.54
1:A:275:LYS:O	1:A:275:LYS:HD3	2.07	0.54
1:B:278:ALA:CB	1:B:357:ARG:HH11	2.20	0.54
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.38	0.54
1:B:269:PRO:O	1:B:270:LEU:O	2.26	0.54
1:B:262:ILE:O	1:B:262:ILE:HG22	2.07	0.53
1:A:436:LEU:O	1:A:439:MET:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLN:O	1:A:280:ARG:NH2	2.42	0.53
1:A:456:ILE:HG21	1:A:463:MET:HE1	1.91	0.53
1:A:437:GLN:O	1:A:440:THR:HG23	2.09	0.52
1:A:463:MET:HE3	1:A:465:LEU:HD21	1.90	0.52
1:B:349:THR:HG23	3:B:1068:HOH:O	2.08	0.52
1:B:270:LEU:HD22	1:B:469:LEU:HD22	1.91	0.52
1:A:263:LYS:NZ	1:A:265:LYS:HE2	2.25	0.52
1:B:402:ASN:O	1:B:405:PRO:HD2	2.09	0.52
1:B:427:GLU:N	1:B:427:GLU:OE2	2.38	0.52
1:A:252:MET:CE	1:A:255:LEU:HD12	2.40	0.52
1:B:349:THR:HG21	3:B:1081:HOH:O	2.09	0.52
1:A:252:MET:HA	1:A:252:MET:CE	2.39	0.51
1:A:354:LYS:HA	1:A:361:GLY:O	2.10	0.51
1:B:257:MET:CG	1:B:261:LYS:HG3	2.41	0.51
1:B:334:MET:HE2	1:B:368:PHE:CE1	2.45	0.51
1:B:342:SER:H	2:B:2:PTG:H20	1.75	0.51
1:B:264:PHE:HB2	1:B:267:ILE:HG12	1.93	0.50
1:A:263:LYS:HD2	1:A:265:LYS:HG2	1.92	0.50
1:A:443:ARG:HG3	1:A:443:ARG:HH11	1.75	0.50
1:B:255:LEU:O	1:B:259:GLU:HG3	2.11	0.50
1:B:329:MET:HB2	3:B:1109:HOH:O	2.12	0.50
1:B:357:ARG:NH2	1:B:358:LYS:CD	2.75	0.50
1:B:466:HIS:CD2	1:B:467:PRO:HD2	2.47	0.50
1:A:443:ARG:NH1	1:B:440:THR:CG2	2.75	0.50
1:B:269:PRO:C	1:B:270:LEU:O	2.55	0.50
1:B:276:GLU:OE2	1:B:276:GLU:C	2.54	0.50
1:A:277:VAL:O	1:A:281:ILE:HG12	2.11	0.50
1:B:362:ASP:CG	1:B:362:ASP:O	2.55	0.49
1:A:443:ARG:NH1	1:B:440:THR:HG21	2.28	0.49
1:A:446:VAL:O	1:A:450:VAL:HG23	2.12	0.49
1:B:207:GLU:C	1:B:209:ALA:H	2.20	0.49
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.95	0.49
1:A:277:VAL:HG13	1:A:278:ALA:N	2.28	0.49
1:A:473:TYR:HA	1:A:476:LEU:HD12	1.95	0.49
1:A:353:LEU:O	1:A:356:LEU:HG	2.12	0.48
1:A:258:GLY:O	1:A:262:ILE:N	2.42	0.48
1:A:264:PHE:O	1:A:266:HIS:N	2.46	0.48
1:B:276:GLU:OE1	1:B:357:ARG:NH2	2.47	0.48
1:A:281:ILE:HD12	1:A:348:MET:HE1	1.96	0.48
1:B:272:GLU:C	1:B:273:GLN:CD	2.82	0.48
1:B:425:HIS:N	1:B:426:PRO:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:HIS:CD2	1:B:468:LEU:H	2.29	0.47
1:B:247:PHE:HB2	1:B:262:ILE:HD12	1.95	0.47
1:B:268:THR:OG1	1:B:270:LEU:CG	2.60	0.47
1:A:272:GLU:HG2	1:A:273:GLN:N	2.18	0.47
1:A:394:SER:O	1:A:397:ARG:HG2	2.15	0.47
1:B:335:ASN:ND2	1:B:337:ASP:N	2.58	0.47
1:A:263:LYS:HE3	1:A:263:LYS:HB3	1.62	0.46
1:B:358:LYS:CB	1:B:359:PRO:HD3	2.39	0.46
1:B:342:SER:H	2:B:2:PTG:C21	2.28	0.46
1:A:289:SER:OG	2:A:1:PTG:H19	2.16	0.46
1:A:443:ARG:HG3	1:A:443:ARG:NH1	2.30	0.46
1:B:357:ARG:HG2	1:B:358:LYS:N	2.30	0.46
1:A:263:LYS:HZ2	1:A:265:LYS:HE2	1.79	0.46
1:B:249:ILE:HD11	1:B:264:PHE:CE1	2.51	0.46
1:B:357:ARG:HD2	3:B:1078:HOH:O	2.15	0.46
1:A:203:GLN:OE1	1:A:203:GLN:O	2.33	0.46
1:B:263:LYS:O	1:B:264:PHE:C	2.59	0.45
1:B:274:SER:CB	1:B:280:ARG:HD3	2.46	0.45
1:B:241:THR:O	1:B:242:THR:C	2.59	0.45
1:B:207:GLU:C	1:B:209:ALA:N	2.72	0.45
1:B:270:LEU:HB3	1:B:273:GLN:OE1	2.16	0.45
1:B:273:GLN:CD	1:B:273:GLN:N	2.74	0.45
1:B:265:LYS:O	1:B:266:HIS:CG	2.70	0.45
1:B:456:ILE:HG22	1:B:456:ILE:O	2.17	0.45
1:A:280:ARG:HD3	1:A:280:ARG:HA	1.89	0.45
1:B:330:LEU:HD22	2:B:2:PTG:H4A	1.98	0.45
1:B:342:SER:H	2:B:2:PTG:H21A	1.83	0.44
1:A:317:LEU:HD22	1:A:392:ILE:O	2.17	0.44
1:B:334:MET:HE2	1:B:368:PHE:CD1	2.52	0.44
1:B:277:VAL:HG12	1:B:278:ALA:N	2.33	0.44
1:B:402:ASN:OD1	1:B:405:PRO:HD3	2.18	0.44
1:B:365:GLU:HB3	1:B:366:PRO:HD3	1.99	0.44
1:A:272:GLU:CG	1:A:273:GLN:N	2.71	0.44
1:A:424:ASN:C	1:A:426:PRO:HD3	2.42	0.44
1:B:217:HIS:HE1	1:B:302:SER:O	2.01	0.44
1:B:403:VAL:HG12	1:B:407:GLU:HG3	2.00	0.44
1:A:358:LYS:CB	1:A:359:PRO:CD	2.96	0.44
1:B:343:GLU:H	2:B:2:PTG:C22	2.31	0.44
1:B:270:LEU:CB	1:B:273:GLN:OE1	2.66	0.43
1:B:357:ARG:CG	1:B:358:LYS:N	2.81	0.43
1:A:255:LEU:HD11	1:A:277:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASP:O	1:B:415:GLN:HG3	2.19	0.43
1:B:466:HIS:CD2	1:B:466:HIS:C	2.97	0.43
1:A:271:GLN:HB2	1:A:280:ARG:HH22	1.84	0.43
1:A:261:LYS:N	1:A:261:LYS:HD2	2.33	0.43
1:A:404:LYS:N	1:A:405:PRO:HD2	2.33	0.43
1:A:234:ARG:NH1	3:A:1009:HOH:O	2.51	0.43
1:B:444:GLN:O	1:B:448:GLU:HB2	2.18	0.43
1:B:425:HIS:HB3	1:B:428:SER:OG	2.18	0.43
1:A:360:PHE:O	1:A:363:PHE:HD2	2.02	0.43
1:A:215:ALA:CB	1:A:386:ILE:HD11	2.48	0.42
1:A:384:LEU:O	1:A:388:ILE:HG13	2.18	0.42
1:B:224:LYS:O	1:B:224:LYS:HG2	2.18	0.42
1:B:393:LEU:HD22	1:B:393:LEU:N	2.34	0.42
1:B:266:HIS:C	1:B:268:THR:HG22	2.44	0.42
1:B:268:THR:C	1:B:270:LEU:H	2.27	0.42
1:B:342:SER:H	2:B:2:PTG:C20	2.32	0.42
1:B:257:MET:HG3	1:B:261:LYS:HG3	2.01	0.42
1:A:252:MET:HE2	1:A:255:LEU:HD12	2.02	0.42
1:A:290:VAL:HG13	1:A:468:LEU:HD23	2.01	0.42
1:A:325:ILE:HD11	1:A:392:ILE:HG13	2.01	0.42
1:A:356:LEU:HD23	1:A:356:LEU:HA	1.81	0.42
1:B:397:ARG:HB2	1:B:400:LEU:HD11	2.00	0.42
1:A:269:PRO:O	1:A:270:LEU:C	2.62	0.42
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.85	0.42
1:B:341:ILE:HA	2:B:2:PTG:H21A	2.01	0.42
1:A:283:GLN:O	1:A:286:GLN:HB2	2.20	0.42
1:B:264:PHE:HD1	1:B:267:ILE:HG13	1.85	0.42
1:B:424:ASN:ND2	3:B:1086:HOH:O	2.53	0.42
1:B:457:LYS:O	1:B:458:LYS:C	2.63	0.42
1:A:265:LYS:H	1:A:265:LYS:HG3	1.49	0.42
1:B:472:ILE:HB	1:B:473:TYR:CD2	2.55	0.42
1:B:311:LEU:N	1:B:311:LEU:CD2	2.79	0.41
1:B:330:LEU:HD21	1:B:364:MET:HE1	2.02	0.41
1:A:204:LEU:HB3	1:A:205:ASN:H	1.38	0.41
1:A:271:GLN:CB	1:A:280:ARG:NH2	2.83	0.41
1:A:288:ARG:HD2	1:A:288:ARG:C	2.45	0.41
1:B:309:LEU:CD2	1:B:405:PRO:HB2	2.50	0.41
1:B:257:MET:HG2	1:B:261:LYS:HG3	2.01	0.41
1:B:282:PHE:HZ	1:B:453:LEU:HD23	1.84	0.41
1:B:245:SER:HA	1:B:246:PRO:HD3	1.92	0.41
1:B:288:ARG:HD2	1:B:288:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:O	1:A:357:ARG:HB2	2.20	0.41
1:A:263:LYS:O	1:A:265:LYS:HG3	2.20	0.41
1:A:268:THR:HG22	1:A:280:ARG:HH11	1.83	0.41
1:B:330:LEU:O	1:B:334:MET:HG3	2.21	0.41
1:A:325:ILE:HD11	1:A:392:ILE:HG12	2.03	0.41
1:B:226:PHE:CG	1:B:329:MET:HE1	2.56	0.41
1:A:463:MET:HE3	1:A:465:LEU:CD2	2.50	0.41
1:B:239:GLY:C	1:B:241:THR:H	2.28	0.41
1:B:349:THR:HG23	1:B:351:GLU:H	1.86	0.41
1:B:356:LEU:O	1:B:361:GLY:HA3	2.21	0.41
1:B:358:LYS:HB3	1:B:359:PRO:HD2	1.93	0.40
1:B:466:HIS:HA	1:B:467:PRO:HD3	1.85	0.40
1:B:322:VAL:O	1:B:326:ILE:HG13	2.21	0.40
1:A:267:ILE:HG22	1:A:284:GLY:O	2.22	0.40
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.57	0.40
1:A:424:ASN:HB3	1:A:425:HIS:ND1	2.36	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	272/286 (95%)	251 (92%)	11 (4%)	10 (4%)	2	0
1	B	259/286 (91%)	232 (90%)	17 (7%)	10 (4%)	2	0
All	All	531/572 (93%)	483 (91%)	28 (5%)	20 (4%)	2	0

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	LYS
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	272	GLU
1	A	358	LYS
1	B	243	ASP
1	B	270	LEU
1	B	274	SER
1	B	358	LYS
1	A	271	GLN
1	A	274	SER
1	B	240	LYS
1	B	265	LYS
1	B	269	PRO
1	B	276	GLU
1	B	460	GLU
1	A	264	PHE
1	A	266	HIS
1	A	357	ARG
1	A	361	GLY
1	B	268	THR

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	247/257 (96%)	233 (94%)	14 (6%)	18	11
1	B	236/257 (92%)	223 (94%)	13 (6%)	19	11
All	All	483/514 (94%)	456 (94%)	27 (6%)	19	11

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	MET
1	A	255	LEU
1	A	257	MET
1	A	268	THR
1	A	269	PRO

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Mol	Chain	Res	Type
1	A	273	GLN
1	A	283	GLN
1	A	311	LEU
1	A	333	LEU
1	A	358	LYS
1	A	427	GLU
1	A	440	THR
1	A	459	THR
1	A	469	LEU
1	B	241	THR
1	B	242	THR
1	B	261	LYS
1	B	268	THR
1	B	273	GLN
1	B	276	GLU
1	B	290	VAL
1	B	335	ASN
1	B	349	THR
1	B	357	ARG
1	B	424	ASN
1	B	427	GLU
1	B	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	271	GLN
1	A	273	GLN
1	A	283	GLN
1	A	308	ASN
1	A	312	ASN
1	A	314	GLN
1	A	323	HIS
1	A	345	GLN
1	A	410	GLN
1	A	425	HIS
1	A	449	HIS
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	283	GLN

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Mol	Chain	Res	Type
1	B	308	ASN
1	B	335	ASN
1	B	424	ASN
1	B	430	GLN
1	B	451	GLN
1	B	454	GLN
1	B	466	HIS
1	B	470	GLN

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](#)

2 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	PTG	B	2	-	21,23,23	1.45	4 (19%)	18,27,27	1.19	3 (16%)
2	PTG	A	1	-	21,23,23	1.52	4 (19%)	18,27,27	1.45	4 (22%)

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	PTG	B	2	-	-	7/17/30/30	0/1/1/1
2	PTG	A	1	-	-	4/17/30/30	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	PTG	C15-C10	-3.97	1.46	1.54
2	A	1	PTG	C15-C10	-3.78	1.47	1.54
2	A	1	PTG	C7-C8	3.55	1.54	1.43
2	B	2	PTG	C7-C8	2.97	1.52	1.43
2	A	1	PTG	O12-C11	2.71	1.31	1.24
2	B	2	PTG	C16-C17	2.62	1.57	1.50
2	A	1	PTG	C16-C17	2.48	1.57	1.50
2	B	2	PTG	O12-C11	2.43	1.31	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	PTG	C8-C10-C11	3.08	122.55	119.72
2	A	1	PTG	O24-C22-C21	2.61	122.24	114.00
2	B	2	PTG	O24-C22-C21	2.43	121.67	114.00
2	A	1	PTG	C8-C7-C6	2.41	129.27	123.63
2	A	1	PTG	O23-C22-C21	-2.38	115.55	123.09
2	B	2	PTG	O23-C22-C21	-2.20	116.11	123.09
2	B	2	PTG	C21-C20-C19	-2.02	108.95	113.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	PTG	C2-C3-C4-C5
2	B	2	PTG	C2-C3-C4-C5
2	A	1	PTG	C1-C2-C3-C4
2	B	2	PTG	C18-C19-C20-C21
2	B	2	PTG	C1-C2-C3-C4
2	B	2	PTG	C14-C15-C16-C17
2	B	2	PTG	C15-C16-C17-C18
2	A	1	PTG	C20-C21-C22-O23
2	A	1	PTG	C20-C21-C22-O24

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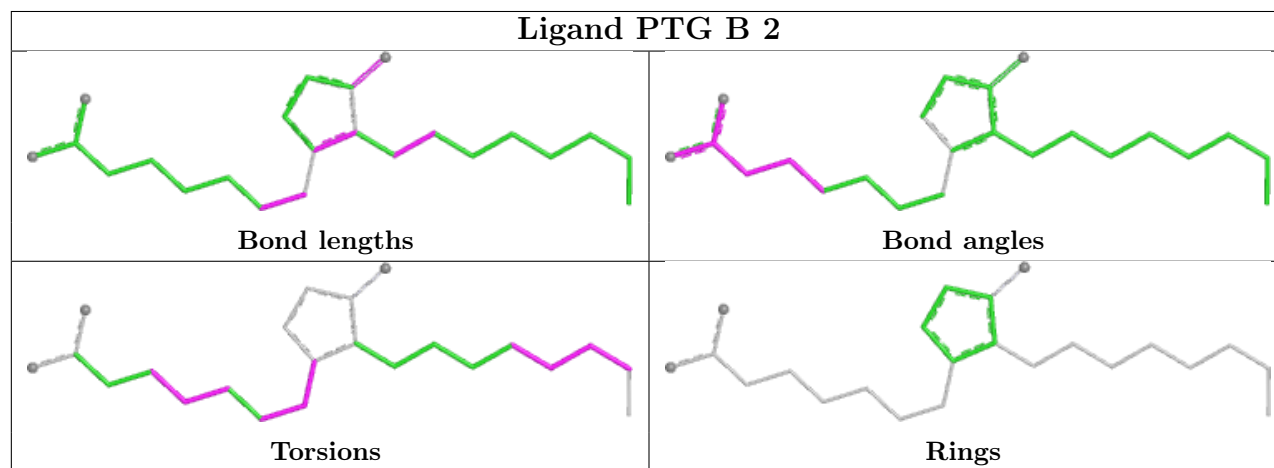
Mol	Chain	Res	Type	Atoms
2	B	2	PTG	C17-C18-C19-C20
2	B	2	PTG	C3-C4-C5-C6

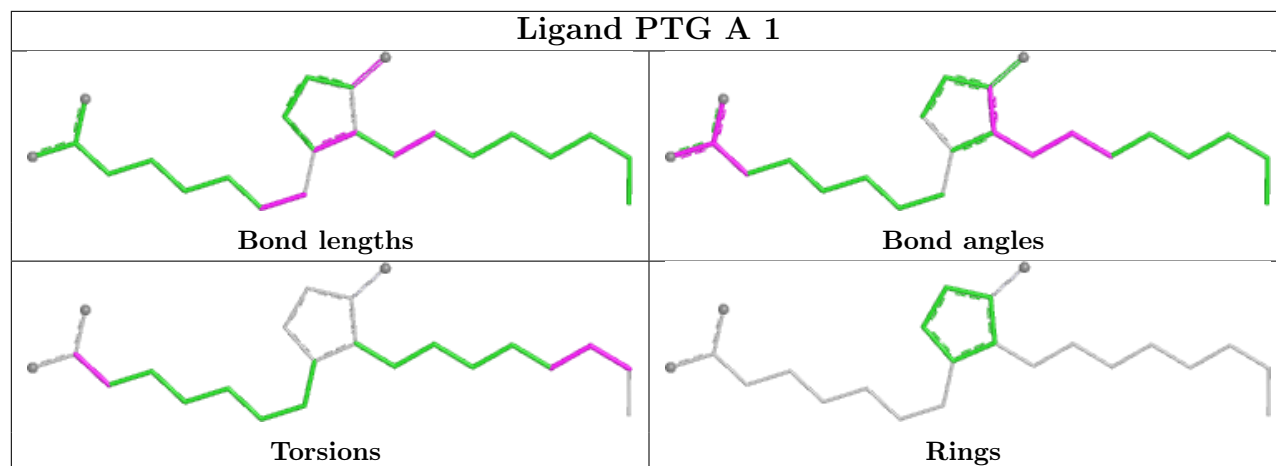
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	PTG	10	0
2	A	1	PTG	2	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	274/286 (95%)	1.20	54 (19%) 3 3	26, 38, 64, 68	0
1	B	263/286 (91%)	1.14	47 (17%) 3 3	24, 38, 61, 68	0
All	All	537/572 (93%)	1.17	101 (18%) 3 3	24, 38, 63, 68	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	PRO	9.9
1	B	241	THR	7.7
1	B	268	THR	7.0
1	A	267	ILE	7.0
1	A	268	THR	6.8
1	A	204	LEU	6.3
1	B	459	THR	5.7
1	B	267	ILE	5.4
1	B	242	THR	5.3
1	B	469	LEU	5.2
1	A	239	GLY	5.1
1	A	270	LEU	4.9
1	A	241	THR	4.7
1	B	274	SER	4.5
1	B	269	PRO	4.5
1	A	453	LEU	4.5
1	B	458	LYS	4.4
1	A	266	HIS	4.1
1	B	273	GLN	4.0
1	B	243	ASP	3.9
1	A	264	PHE	3.9
1	A	277	VAL	3.9
1	A	262	ILE	3.9
1	B	264	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	266	HIS	3.7
1	B	363	PHE	3.6
1	B	239	GLY	3.6
1	A	253	ASN	3.5
1	B	256	MET	3.5
1	A	476	LEU	3.5
1	A	359	PRO	3.4
1	A	261	LYS	3.4
1	A	265	LYS	3.4
1	A	356	LEU	3.4
1	B	450	VAL	3.3
1	A	444	GLN	3.3
1	A	362	ASP	3.3
1	B	270	LEU	3.2
1	A	242	THR	3.2
1	B	262	ILE	3.2
1	A	252	MET	3.2
1	B	209	ALA	3.1
1	B	455	VAL	3.1
1	B	452	LEU	3.0
1	A	243	ASP	3.0
1	A	256	MET	2.9
1	A	238	THR	2.8
1	A	363	PHE	2.8
1	B	272	GLU	2.8
1	A	273	GLN	2.7
1	A	360	PHE	2.7
1	A	272	GLU	2.7
1	A	411	ASP	2.7
1	A	358	LYS	2.7
1	A	275	LYS	2.7
1	B	428	SER	2.6
1	A	426	PRO	2.6
1	A	287	PHE	2.6
1	B	260	ASP	2.6
1	B	258	GLY	2.6
1	B	343	GLU	2.5
1	A	257	MET	2.5
1	B	456	ILE	2.5
1	B	265	LYS	2.4
1	B	461	THR	2.4
1	A	440	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	280	ARG	2.4
1	A	427	GLU	2.4
1	B	208	SER	2.4
1	B	232	LYS	2.4
1	B	470	GLN	2.4
1	A	271	GLN	2.3
1	A	342	SER	2.3
1	A	205	ASN	2.3
1	B	358	LYS	2.3
1	B	254	SER	2.3
1	B	359	PRO	2.3
1	A	279	ILE	2.3
1	B	357	ARG	2.3
1	A	475	ASP	2.3
1	A	263	LYS	2.2
1	B	238	THR	2.2
1	A	361	GLY	2.2
1	A	388	ILE	2.2
1	B	453	LEU	2.2
1	A	474	LYS	2.2
1	A	357	ARG	2.2
1	B	451	GLN	2.2
1	B	454	GLN	2.1
1	A	311	LEU	2.1
1	B	457	LYS	2.1
1	A	260	ASP	2.1
1	B	210	ASP	2.1
1	B	447	THR	2.1
1	B	473	TYR	2.1
1	B	240	LYS	2.0
1	A	439	MET	2.0
1	B	468	LEU	2.0
1	A	274	SER	2.0
1	A	464	SER	2.0
1	A	459	THR	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 [i](#)

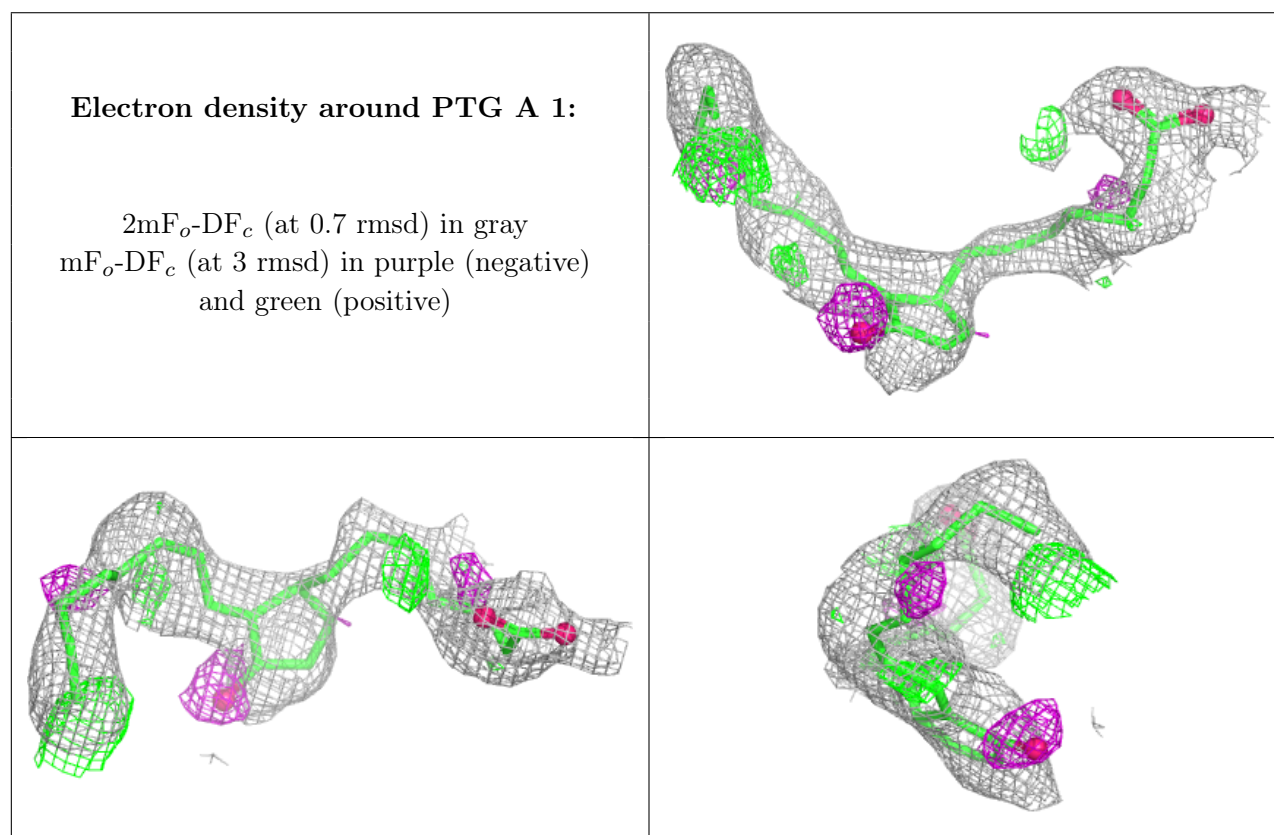
There are no oligosaccharides in this entry.

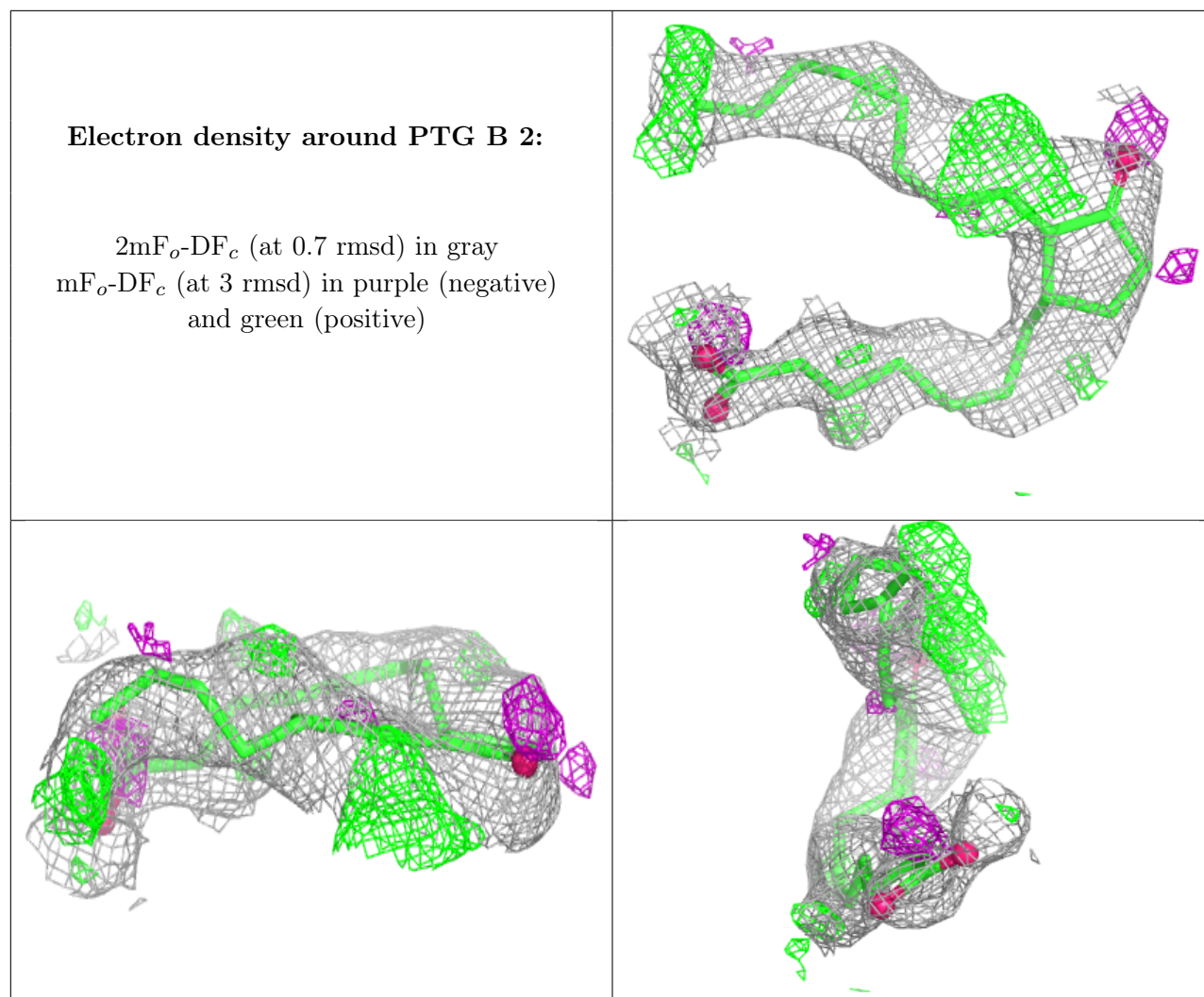
6.4 Ligands [i](#)

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
2	PTG	A	1	23/23	0.57	0.23	53,60,61,63	0
2	PTG	B	2	23/23	0.61	0.25	49,58,62,64	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.