



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:58 pm BST

PDB ID : 2ZK2  
Title : Human peroxisome proliferator-activated receptor gamma ligand binding domain complexed with glutathion conjugated 15-deoxy-delta12,14-prostaglandin J2  
Authors : Waku, T.; Shiraki, T.; Oyama, T.; Fujimoto, Y.; Morikawa, K.  
Deposited on : 2008-03-12  
Resolution : 2.26 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

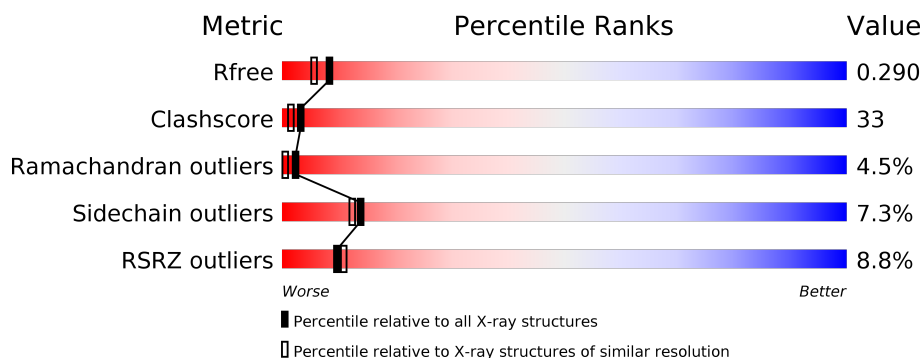
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.26 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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>5%</div> <div> <div></div> <div>52%</div> <div>36%</div> <div>7%</div> <div></div> </div> </div>
1	B	286	<div> <div>11%</div> <div> <div></div> <div>49%</div> <div>35%</div> <div>6%</div> <div>8%</div> </div> </div>

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
3	PTG	A	477	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4424 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.

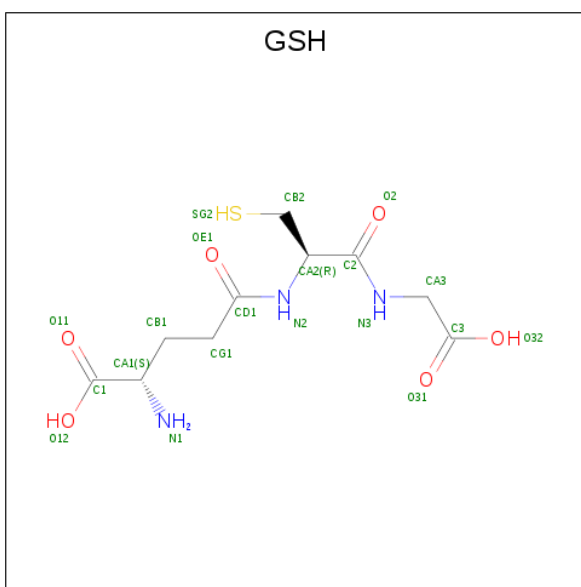
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2186	1409	358	409	10			
1	B	263	Total	C	N	O	S	0	0	0
			2110	1363	346	392	9			

There are 8 discrepancies between the modelled and reference sequences:

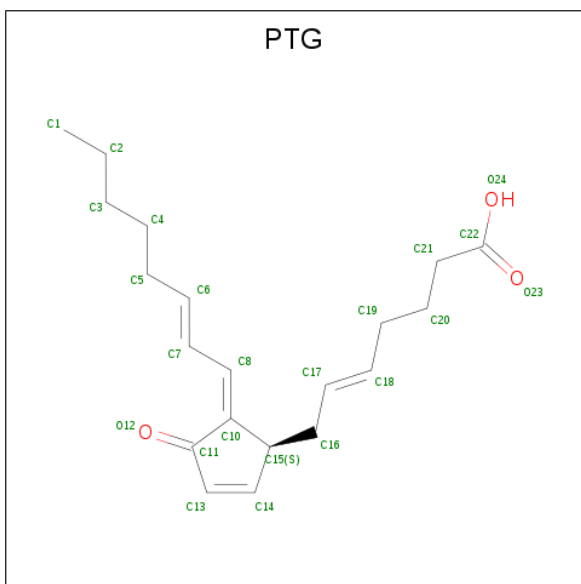
Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	EXPRESSION TAG	UNP P37231
A	192	SER	-	EXPRESSION TAG	UNP P37231
A	193	HIS	-	EXPRESSION TAG	UNP P37231
A	194	MET	-	EXPRESSION TAG	UNP P37231
B	191	GLY	-	EXPRESSION TAG	UNP P37231
B	192	SER	-	EXPRESSION TAG	UNP P37231
B	193	HIS	-	EXPRESSION TAG	UNP P37231
B	194	MET	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is (5E,14E)-11-oxoprostano-5,9,12,14-tetraen-1-oic acid (three-letter code: PTG) (formula:  $C_{20}H_{28}O_3$ ).



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

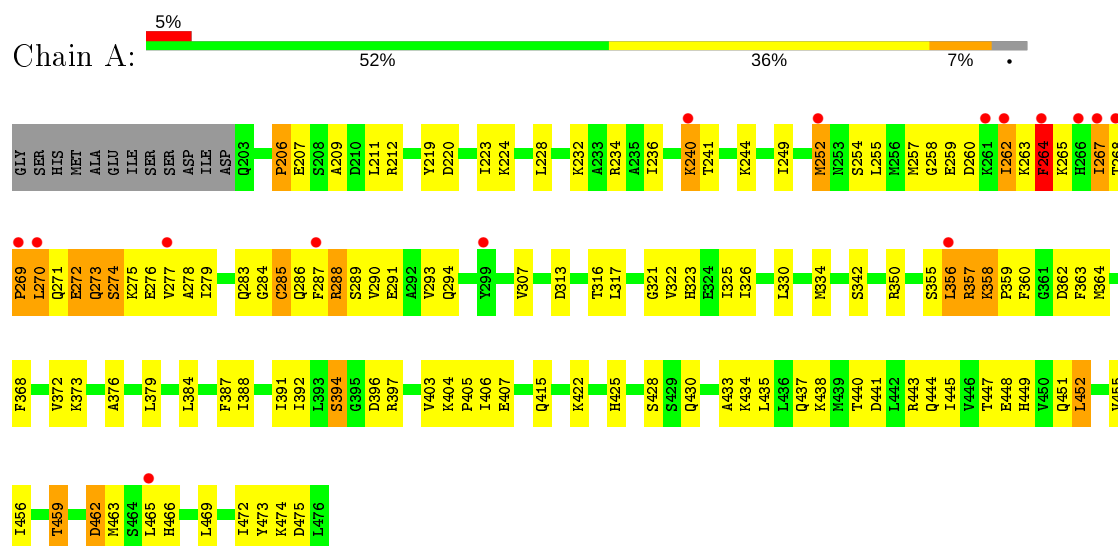
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total 54	O 54	0	0
4	B	31	Total 31	O 31	0	0

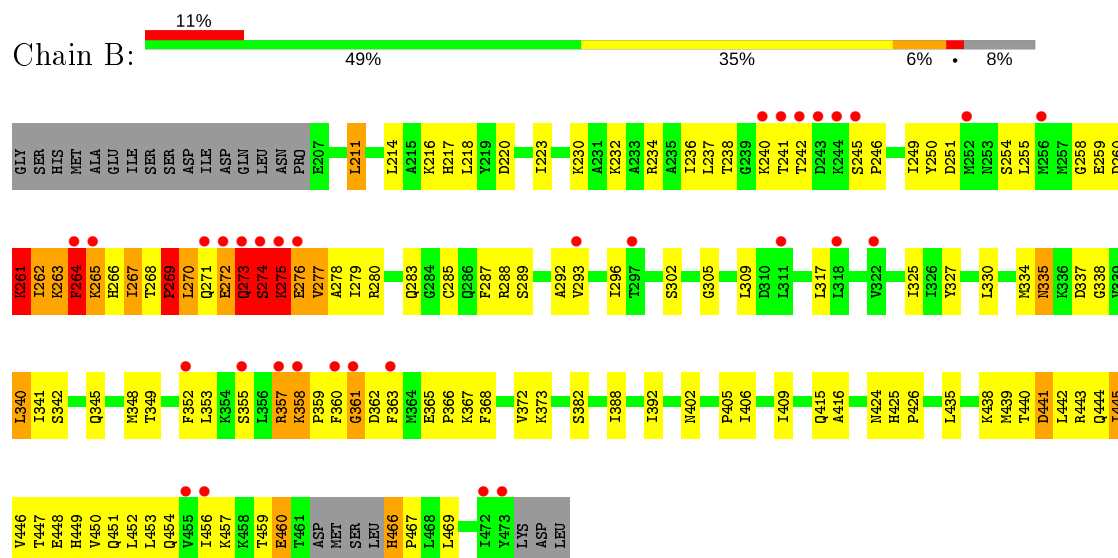
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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, $\alpha$ , $\beta$ , $\gamma$	93.38 Å   61.35 Å   118.69 Å 90.00°   103.02°   90.00°	Depositor
Resolution (Å)	48.88 – 2.26 48.88 – 2.26	Depositor EDS
% Data completeness (in resolution range)	93.0 (48.88-2.26) 93.1 (48.88-2.26)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.27 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.247   ,   0.299 0.240   ,   0.290	Depositor DCC
$R_{free}$ test set	1495 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.2	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PTG, GSH

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	0.43	0/2223	0.68	3/2995 (0.1%)
1	B	0.43	0/2146	0.66	0/2891
All	All	0.43	0/4369	0.67	3/5886 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	264	PHE	N-CA-C	5.58	126.06	111.00
1	A	206	PRO	N-CA-CB	5.15	109.48	103.30
1	A	272	GLU	N-CA-C	-5.02	97.45	111.00

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	2186	0	2238	142	0
1	B	2110	0	2174	156	0
2	A	20	0	14	5	0
3	A	23	0	25	11	0
4	A	54	0	0	3	0
4	B	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4424	0	4451	289	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 33.

All (289) 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:241:THR:HG21	1:A:244:LYS:HD2	1.33	1.09
1:B:358:LYS:HB3	1:B:359:PRO:CD	1.82	1.08
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.29	1.05
1:B:459:THR:HG22	1:B:460:GLU:H	1.26	1.00
1:A:252:MET:HE1	1:A:277:VAL:HG21	1.43	0.98
1:A:211:LEU:HD11	1:A:415:GLN:HE21	1.23	0.97
1:B:259:GLU:HB3	1:B:265:LYS:HE2	1.48	0.95
1:B:259:GLU:O	1:B:263:LYS:HA	1.74	0.88
1:B:234:ARG:O	1:B:238:THR:HG22	1.74	0.87
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.55	0.86
1:A:291:GLU:HA	1:A:294:GLN:OE1	1.77	0.85
1:B:335:ASN:HD22	1:B:335:ASN:C	1.80	0.84
1:B:268:THR:O	1:B:270:LEU:N	2.12	0.82
1:A:274:SER:O	1:A:276:GLU:N	2.11	0.82
1:B:265:LYS:HG3	1:B:269:PRO:HD3	1.61	0.82
1:B:453:LEU:O	1:B:456:ILE:HG22	1.80	0.82
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.64	0.79
1:A:441:ASP:O	1:A:445:ILE:HG12	1.81	0.79
1:B:276:GLU:H	1:B:280:ARG:HH21	1.28	0.79
1:B:276:GLU:H	1:B:280:ARG:NH2	1.82	0.78
1:B:335:ASN:ND2	1:B:338:GLY:H	1.82	0.78
1:A:252:MET:HE3	1:A:252:MET:HA	1.66	0.77
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.65	0.77
1:B:466:HIS:HA	1:B:469:LEU:HD12	1.67	0.76
1:B:267:ILE:HG22	1:B:287:PHE:CB	2.16	0.75
1:A:278:ALA:HA	1:A:356:LEU:HD22	1.68	0.73
1:B:273:GLN:HE22	1:B:280:ARG:HD3	1.54	0.73
1:B:270:LEU:CD1	1:B:273:GLN:HG2	2.18	0.73
1:B:263:LYS:C	1:B:265:LYS:H	1.91	0.73
1:B:249:ILE:HA	1:B:254:SER:HB3	1.71	0.72
1:A:267:ILE:HG22	1:A:268:THR:N	2.04	0.72
1:A:443:ARG:HH11	1:B:444:GLN:HE22	1.38	0.72
1:B:335:ASN:ND2	1:B:337:ASP:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:HA	1:A:267:ILE:HD13	1.72	0.71
1:A:363:PHE:CE1	1:A:452:LEU:HD22	2.25	0.71
1:B:267:ILE:HG22	1:B:287:PHE:HB3	1.72	0.70
1:A:313:ASP:HA	1:A:316:THR:HG22	1.72	0.70
1:A:211:LEU:HD11	1:A:415:GLN:NE2	2.02	0.70
1:A:252:MET:HA	1:A:252:MET:CE	2.22	0.69
1:A:240:LYS:HB3	1:A:240:LYS:NZ	2.06	0.69
1:A:264:PHE:HD1	1:A:264:PHE:O	1.74	0.69
1:A:267:ILE:HG13	1:A:288:ARG:HD3	1.74	0.69
1:B:266:HIS:O	1:B:269:PRO:HD2	1.93	0.69
1:A:273:GLN:HG3	1:A:274:SER:N	2.09	0.68
1:A:455:VAL:O	1:A:459:THR:HG22	1.94	0.68
1:B:214:LEU:O	1:B:218:LEU:HG	1.95	0.67
1:B:273:GLN:HE21	1:B:274:SER:CA	2.08	0.67
1:B:402:ASN:O	1:B:405:PRO:HD2	1.95	0.66
1:A:394:SER:HB2	1:A:397:ARG:HG2	1.78	0.66
1:A:272:GLU:O	1:A:273:GLN:HB3	1.95	0.66
2:A:1:GSH:HB22	3:A:477:PTG:H16	1.77	0.65
1:A:355:SER:O	1:A:357:ARG:N	2.30	0.65
1:A:262:ILE:HD11	1:A:264:PHE:CE2	2.32	0.65
1:B:368:PHE:O	1:B:372:VAL:HG23	1.96	0.65
1:A:262:ILE:HD11	1:A:264:PHE:HE2	1.59	0.65
1:B:363:PHE:CE1	1:B:452:LEU:HB3	2.32	0.65
1:B:358:LYS:CB	1:B:359:PRO:CD	2.70	0.64
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.79	0.64
1:A:259:GLU:HG2	1:A:264:PHE:HE1	1.63	0.64
1:B:459:THR:HG22	1:B:460:GLU:N	2.06	0.64
1:B:270:LEU:HD13	1:B:273:GLN:HG2	1.79	0.63
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.28	0.63
1:A:289:SER:OG	3:A:477:PTG:H3	1.99	0.63
1:B:296:ILE:HD12	1:B:325:ILE:HG21	1.80	0.63
1:B:466:HIS:HA	1:B:469:LEU:HB2	1.80	0.63
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.80	0.62
1:B:330:LEU:O	1:B:334:MET:HG3	1.99	0.62
1:A:284:GLY:HA3	2:A:1:GSH:O12	2.00	0.62
1:A:326:ILE:HG23	3:A:477:PTG:H18	1.81	0.62
1:B:266:HIS:C	1:B:269:PRO:HD2	2.19	0.62
1:B:273:GLN:HE21	1:B:274:SER:N	1.98	0.62
1:A:264:PHE:O	1:A:264:PHE:CD1	2.54	0.61
1:A:357:ARG:HG2	1:A:358:LYS:H	1.66	0.61
1:B:263:LYS:O	1:B:265:LYS:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:GLU:O	1:B:451:GLN:N	2.32	0.61
1:B:349:THR:HG23	1:B:352:PHE:H	1.63	0.61
1:B:262:ILE:HG22	1:B:345:GLN:HB3	1.83	0.61
1:A:313:ASP:HA	1:A:316:THR:CG2	2.31	0.61
1:A:270:LEU:HG	1:A:270:LEU:O	2.00	0.60
1:B:292:ALA:O	1:B:296:ILE:HG12	2.01	0.60
1:A:240:LYS:O	1:A:241:THR:HG23	2.01	0.60
1:A:234:ARG:HH11	1:A:234:ARG:HG3	1.66	0.60
1:A:387:PHE:CE2	1:A:391:ILE:HD11	2.37	0.60
1:A:368:PHE:O	1:A:372:VAL:HG23	2.01	0.59
1:B:348:MET:SD	1:B:353:LEU:HD21	2.43	0.59
1:A:286:GLN:HE22	1:A:465:LEU:HD23	1.67	0.59
1:A:240:LYS:O	1:A:241:THR:CG2	2.51	0.59
1:A:449:HIS:NE2	3:A:477:PTG:H1A	2.18	0.59
1:A:272:GLU:OE1	1:A:273:GLN:HG2	2.03	0.58
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.38	0.58
1:A:462:ASP:N	1:A:462:ASP:OD1	2.35	0.58
1:B:335:ASN:C	1:B:335:ASN:ND2	2.52	0.58
1:B:261:LYS:C	1:B:263:LYS:N	2.55	0.58
1:B:216:LYS:HE3	1:B:220:ASP:OD1	2.02	0.58
1:B:258:GLY:O	1:B:262:ILE:HG12	2.03	0.58
1:B:276:GLU:N	1:B:280:ARG:HH21	2.00	0.58
1:B:441:ASP:OD1	1:B:441:ASP:N	2.35	0.58
1:B:273:GLN:O	1:B:275:LYS:N	2.35	0.57
1:B:267:ILE:HG13	1:B:268:THR:HG23	1.85	0.57
1:A:357:ARG:CG	1:A:358:LYS:H	2.17	0.57
1:A:270:LEU:C	1:A:271:GLN:HG2	2.24	0.57
1:B:268:THR:HG22	1:B:280:ARG:HG2	1.85	0.57
1:B:277:VAL:HG13	1:B:278:ALA:H	1.69	0.57
1:B:265:LYS:HG3	1:B:269:PRO:CD	2.33	0.57
1:A:433:ALA:O	1:A:437:GLN:HG3	2.05	0.56
1:A:323:HIS:CD2	1:A:473:TYR:HH	2.23	0.56
1:B:363:PHE:O	1:B:366:PRO:HD2	2.04	0.56
1:A:443:ARG:HH11	1:B:444:GLN:NE2	2.04	0.56
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.35	0.56
1:A:265:LYS:HD3	1:A:265:LYS:O	2.06	0.56
1:B:273:GLN:HE22	1:B:280:ARG:CD	2.18	0.56
1:B:360:PHE:C	1:B:362:ASP:H	2.09	0.56
1:A:323:HIS:CE1	1:A:472:ILE:HG21	2.41	0.56
1:B:363:PHE:CD1	1:B:452:LEU:HD23	2.40	0.56
1:A:443:ARG:NH1	1:B:444:GLN:HE22	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LYS:HG3	1:B:262:ILE:N	2.21	0.55
1:A:258:GLY:O	1:A:262:ILE:HG12	2.06	0.55
1:B:335:ASN:ND2	1:B:338:GLY:N	2.53	0.55
1:A:307:VAL:HG22	4:A:1005:HOH:O	2.07	0.55
1:B:268:THR:OG1	1:B:269:PRO:HD3	2.07	0.55
1:B:237:LEU:HD21	1:B:340:LEU:HD13	1.87	0.55
1:A:355:SER:O	1:A:356:LEU:C	2.45	0.55
1:B:262:ILE:O	1:B:264:PHE:N	2.39	0.55
1:B:459:THR:CG2	1:B:460:GLU:H	2.08	0.55
1:A:270:LEU:CG	1:A:270:LEU:O	2.55	0.55
1:A:440:THR:HG22	1:B:440:THR:OG1	2.07	0.55
1:B:255:LEU:CD2	1:B:277:VAL:HG23	2.37	0.55
1:B:335:ASN:HD21	1:B:338:GLY:N	2.05	0.55
1:B:466:HIS:CA	1:B:469:LEU:HD12	2.37	0.55
1:A:268:THR:CG2	1:A:271:GLN:HG3	2.37	0.54
1:B:277:VAL:HG13	1:B:278:ALA:N	2.22	0.54
1:A:357:ARG:CG	1:A:358:LYS:N	2.71	0.54
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.88	0.54
1:B:262:ILE:O	1:B:263:LYS:C	2.44	0.54
1:B:327:TYR:CZ	1:B:367:LYS:NZ	2.75	0.54
1:A:363:PHE:CD2	1:A:452:LEU:HD13	2.43	0.54
1:A:474:LYS:HE3	1:A:475:ASP:OD1	2.08	0.54
1:A:241:THR:HG22	4:A:1019:HOH:O	2.08	0.53
1:A:232:LYS:O	1:A:236:ILE:HG13	2.08	0.53
1:A:364:MET:SD	3:A:477:PTG:H7	2.48	0.53
1:A:443:ARG:NH1	1:B:440:THR:CG2	2.72	0.53
1:A:326:ILE:HA	3:A:477:PTG:H21A	1.91	0.53
1:B:261:LYS:HA	1:B:261:LYS:HE3	1.90	0.53
1:A:287:PHE:CE2	1:A:288:ARG:NH2	2.76	0.53
1:B:268:THR:O	1:B:270:LEU:HD12	2.09	0.53
1:B:273:GLN:NE2	1:B:280:ARG:HD3	2.24	0.53
1:A:293:VAL:HG13	1:A:322:VAL:HG21	1.91	0.52
1:B:443:ARG:O	1:B:447:THR:HG23	2.09	0.52
1:B:270:LEU:HD22	1:B:469:LEU:CD1	2.39	0.52
1:A:241:THR:HG21	1:A:244:LYS:CD	2.23	0.52
1:A:240:LYS:C	1:A:241:THR:HG23	2.30	0.52
1:A:323:HIS:HE1	1:A:472:ILE:HG21	1.74	0.52
1:A:444:GLN:O	1:A:448:GLU:HB3	2.10	0.52
1:B:232:LYS:O	1:B:236:ILE:HG13	2.10	0.52
1:B:450:VAL:HA	1:B:453:LEU:HD12	1.92	0.51
1:B:240:LYS:O	1:B:242:THR:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ASP:O	1:B:254:SER:HB2	2.09	0.51
1:B:341:ILE:HD12	1:B:342:SER:OG	2.11	0.51
1:A:473:TYR:OH	3:A:477:PTG:H1B	2.11	0.51
1:B:262:ILE:C	1:B:264:PHE:N	2.63	0.51
1:A:358:LYS:H	1:A:359:PRO:CD	2.23	0.51
1:A:430:GLN:O	1:A:434:LYS:HG3	2.11	0.51
1:A:404:LYS:HB3	1:A:405:PRO:CD	2.41	0.51
1:A:274:SER:C	1:A:276:GLU:N	2.65	0.51
1:A:473:TYR:HH	3:A:477:PTG:H1B	1.76	0.51
1:B:402:ASN:OD1	1:B:405:PRO:HD3	2.11	0.51
1:B:250:TYR:HA	1:B:349:THR:HG22	1.92	0.51
1:B:466:HIS:O	1:B:469:LEU:N	2.44	0.50
1:A:279:ILE:O	1:A:283:GLN:HG2	2.11	0.50
1:A:396:ASP:HB2	1:B:373:LYS:NZ	2.25	0.50
1:B:317:LEU:HD21	1:B:406:ILE:HD13	1.94	0.50
1:B:452:LEU:O	1:B:456:ILE:HB	2.12	0.50
1:B:250:TYR:HA	1:B:349:THR:CG2	2.41	0.50
1:A:443:ARG:NH1	1:B:440:THR:HG22	2.27	0.50
1:B:251:ASP:OD1	1:B:251:ASP:C	2.50	0.50
1:B:261:LYS:C	1:B:263:LYS:H	2.14	0.50
1:B:296:ILE:HD12	1:B:325:ILE:CG2	2.41	0.50
1:A:277:VAL:HG13	1:A:278:ALA:N	2.27	0.49
1:A:206:PRO:O	1:A:209:ALA:HB3	2.12	0.49
1:A:249:ILE:HG21	1:A:255:LEU:HD23	1.93	0.49
1:A:274:SER:C	1:A:276:GLU:H	2.14	0.49
1:B:275:LYS:NZ	1:B:275:LYS:HB2	2.28	0.49
1:A:264:PHE:CA	1:A:267:ILE:HD13	2.42	0.49
1:A:267:ILE:CG2	1:A:268:THR:N	2.75	0.49
1:A:447:THR:O	1:A:451:GLN:HG3	2.13	0.49
1:A:285:CYS:HB2	3:A:477:PTG:C11	2.42	0.49
1:B:270:LEU:HD22	1:B:469:LEU:HD13	1.94	0.49
1:B:273:GLN:HE21	1:B:274:SER:HA	1.78	0.49
1:B:466:HIS:HB3	1:B:467:PRO:HD3	1.95	0.49
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.43	0.49
1:A:363:PHE:CE2	1:A:452:LEU:HB3	2.48	0.49
1:A:384:LEU:O	1:A:388:ILE:HG12	2.13	0.49
1:A:435:LEU:O	1:A:438:LYS:HB2	2.12	0.48
1:A:387:PHE:O	1:A:391:ILE:HG13	2.14	0.48
1:B:211:LEU:HG	1:B:416:ALA:HA	1.94	0.48
1:B:349:THR:CG2	1:B:352:PHE:HB2	2.44	0.48
1:A:254:SER:O	1:A:258:GLY:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:O	1:B:273:GLN:HB3	2.13	0.48
1:B:273:GLN:HE22	1:B:280:ARG:CG	2.26	0.48
1:A:342:SER:H	2:A:1:GSH:CD1	2.27	0.48
1:A:283:GLN:HE21	1:A:283:GLN:HA	1.78	0.48
1:B:280:ARG:HA	1:B:283:GLN:HE21	1.78	0.47
1:A:321:GLY:HA2	1:A:397:ARG:NH2	2.29	0.47
1:B:276:GLU:O	1:B:278:ALA:N	2.47	0.47
1:A:350:ARG:HG3	1:A:368:PHE:CD2	2.49	0.47
1:B:359:PRO:O	1:B:362:ASP:HB2	2.15	0.47
1:B:255:LEU:HD23	1:B:277:VAL:HG23	1.95	0.47
1:B:267:ILE:CG1	1:B:268:THR:N	2.77	0.47
1:B:360:PHE:O	1:B:362:ASP:N	2.48	0.47
1:B:288:ARG:HD2	1:B:288:ARG:O	2.15	0.47
1:B:358:LYS:CB	1:B:359:PRO:HD3	2.21	0.47
1:B:442:LEU:O	1:B:445:ILE:HG22	2.15	0.47
1:B:230:LYS:O	1:B:234:ARG:HG2	2.15	0.47
1:B:268:THR:O	1:B:269:PRO:C	2.52	0.47
1:B:457:LYS:C	1:B:459:THR:H	2.18	0.46
1:B:442:LEU:O	1:B:446:VAL:HG23	2.14	0.46
1:A:228:LEU:HA	4:A:1076:HOH:O	2.14	0.46
1:A:373:LYS:O	1:A:376:ALA:HB3	2.15	0.46
1:B:360:PHE:C	1:B:362:ASP:N	2.69	0.46
1:A:437:GLN:HG2	1:B:439:MET:HE1	1.98	0.46
1:A:321:GLY:O	1:A:325:ILE:HG13	2.15	0.46
1:A:330:LEU:HD13	3:A:477:PTG:H15	1.97	0.46
1:A:276:GLU:OE1	1:A:357:ARG:CZ	2.64	0.46
1:A:363:PHE:CG	1:A:452:LEU:HD13	2.50	0.46
1:B:263:LYS:C	1:B:265:LYS:N	2.61	0.46
1:B:268:THR:N	1:B:269:PRO:HD2	2.30	0.46
1:B:435:LEU:O	1:B:438:LYS:HB2	2.16	0.45
1:A:240:LYS:HB3	1:A:240:LYS:HZ3	1.76	0.45
1:A:257:MET:O	1:A:260:ASP:HB3	2.17	0.45
1:A:271:GLN:NE2	1:A:273:GLN:O	2.46	0.45
1:B:255:LEU:O	1:B:258:GLY:N	2.49	0.45
1:A:403:VAL:CG1	1:A:407:GLU:OE2	2.65	0.45
1:B:278:ALA:HB3	1:B:357:ARG:HH21	1.81	0.45
1:B:448:GLU:O	1:B:449:HIS:C	2.55	0.45
1:B:305:GLY:HA3	1:B:409:ILE:CD1	2.47	0.45
1:A:267:ILE:O	1:A:269:PRO:HD3	2.17	0.45
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.51	0.45
1:B:277:VAL:H	1:B:280:ARG:NH2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:PHE:CZ	1:B:452:LEU:HB3	2.52	0.45
1:A:422:LYS:HA	1:A:422:LYS:HD2	1.82	0.45
1:B:353:LEU:O	1:B:361:GLY:HA2	2.17	0.45
1:A:317:LEU:HD21	1:A:406:ILE:HD13	1.99	0.44
1:B:335:ASN:HD22	1:B:338:GLY:H	1.62	0.44
1:A:443:ARG:HG3	1:B:444:GLN:HE22	1.82	0.44
1:A:330:LEU:O	1:A:334:MET:HG3	2.18	0.44
1:A:425:HIS:HB3	1:A:428:SER:HB2	1.99	0.44
1:A:276:GLU:OE1	1:A:357:ARG:NH1	2.51	0.44
1:A:236:ILE:HG23	1:A:244:LYS:O	2.18	0.44
1:A:363:PHE:CZ	1:A:452:LEU:HD22	2.52	0.43
1:B:245:SER:HA	1:B:246:PRO:HD3	1.74	0.43
1:B:367:LYS:H	1:B:367:LYS:HG2	1.66	0.43
1:A:267:ILE:HG23	1:A:284:GLY:HA2	2.01	0.43
1:A:287:PHE:CD2	1:A:288:ARG:NE	2.87	0.43
1:B:261:LYS:H	1:B:263:LYS:H	1.66	0.43
1:B:335:ASN:ND2	1:B:337:ASP:N	2.61	0.43
1:B:237:LEU:CD2	1:B:340:LEU:HD13	2.49	0.43
1:B:289:SER:O	1:B:293:VAL:HG23	2.18	0.43
1:A:465:LEU:O	1:A:466:HIS:HB2	2.18	0.43
1:B:273:GLN:NE2	1:B:274:SER:HA	2.34	0.43
2:A:1:GSH:CB2	3:A:477:PTG:H16	2.49	0.42
1:B:365:GLU:HB3	1:B:366:PRO:HD3	2.01	0.42
1:B:325:ILE:HG12	1:B:388:ILE:HG23	2.02	0.42
1:B:445:ILE:O	1:B:445:ILE:HD13	2.19	0.42
1:A:456:ILE:HG21	1:A:463:MET:HE1	2.00	0.42
1:A:360:PHE:C	1:A:362:ASP:H	2.24	0.41
1:A:212:ARG:HA	1:A:212:ARG:HD2	1.89	0.41
1:A:430:GLN:OE1	1:B:415:GLN:HG2	2.20	0.41
1:B:451:GLN:O	1:B:454:GLN:CB	2.69	0.41
1:B:267:ILE:HG22	1:B:287:PHE:CG	2.54	0.41
1:B:405:PRO:O	1:B:409:ILE:HG12	2.21	0.41
1:A:252:MET:HE1	1:A:277:VAL:CG2	2.33	0.41
1:A:211:LEU:HD11	1:A:415:GLN:HG2	2.03	0.41
1:B:276:GLU:HG3	1:B:279:ILE:HB	2.02	0.41
1:A:272:GLU:CD	1:A:272:GLU:O	2.58	0.41
1:A:277:VAL:HG13	1:A:278:ALA:H	1.84	0.41
1:A:396:ASP:HB2	1:B:373:LYS:HZ2	1.86	0.41
1:B:362:ASP:O	1:B:366:PRO:HD3	2.20	0.41
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.39	0.40
1:B:353:LEU:HD12	1:B:368:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:HIS:O	1:B:467:PRO:C	2.58	0.40
1:A:262:ILE:CD1	1:A:264:PHE:CE2	3.03	0.40
1:A:284:GLY:HA3	2:A:1:GSH:C1	2.51	0.40
1:B:363:PHE:CZ	1:B:456:ILE:HD12	2.57	0.40
1:A:379:LEU:HD11	1:A:435:LEU:HD13	2.03	0.40
1:B:217:HIS:HE1	1:B:302:SER:O	2.04	0.40
1:B:223:ILE:HD13	1:B:223:ILE:HA	1.96	0.40
1:B:309:LEU:CD2	1:B:405:PRO:HB2	2.51	0.40
1:A:220:ASP:O	1:A:224:LYS:HG3	2.22	0.40
1:B:425:HIS:N	1:B:426:PRO:HD3	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%)	250 (92%)	11 (4%)	11 (4%)	3	1
1	B	259/286 (91%)	226 (87%)	20 (8%)	13 (5%)	2	0
All	All	531/572 (93%)	476 (90%)	31 (6%)	24 (4%)	2	0

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	LYS
1	A	273	GLN
1	A	275	LYS
1	A	356	LEU
1	B	241	THR
1	B	261	LYS
1	B	269	PRO
1	B	271	GLN

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Mol	Chain	Res	Type
1	B	273	GLN
1	B	276	GLU
1	B	277	VAL
1	A	269	PRO
1	A	270	LEU
1	A	274	SER
1	B	263	LYS
1	B	264	PHE
1	B	275	LYS
1	B	358	LYS
1	A	394	SER
1	B	274	SER
1	A	357	ARG
1	A	267	ILE
1	A	358	LYS
1	B	361	GLY

### 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	243/257 (95%)	232 (96%)	11 (4%)	27	31
1	B	236/257 (92%)	212 (90%)	24 (10%)	7	5
All	All	479/514 (93%)	444 (93%)	35 (7%)	14	12

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	240	LYS
1	A	252	MET
1	A	262	ILE
1	A	264	PHE
1	A	285	CYS
1	A	288	ARG

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Mol	Chain	Res	Type
1	A	452	LEU
1	A	459	THR
1	A	462	ASP
1	A	469	LEU
1	B	211	LEU
1	B	260	ASP
1	B	261	LYS
1	B	262	ILE
1	B	264	PHE
1	B	265	LYS
1	B	267	ILE
1	B	269	PRO
1	B	270	LEU
1	B	272	GLU
1	B	273	GLN
1	B	274	SER
1	B	275	LYS
1	B	285	CYS
1	B	335	ASN
1	B	340	LEU
1	B	355	SER
1	B	357	ARG
1	B	382	SER
1	B	424	ASN
1	B	441	ASP
1	B	445	ILE
1	B	460	GLU
1	B	466	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	HIS
1	A	271	GLN
1	A	273	GLN
1	A	283	GLN
1	A	308	ASN
1	A	415	GLN
1	A	424	ASN
1	A	466	HIS
1	B	217	HIS
1	B	273	GLN

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Mol	Chain	Res	Type
1	B	283	GLN
1	B	314	GLN
1	B	335	ASN
1	B	424	ASN
1	B	430	GLN
1	B	444	GLN
1	B	466	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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
3	PTG	A	477	1,2	16,23,23	1.21	2 (12%)	15,27,27	0.89	1 (6%)
2	GSH	A	1	3	12,19,19	1.30	1 (8%)	15,24,24	2.50	5 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PTG	A	477	1,2	-	5/15/30/30	0/1/1/1
2	GSH	A	1	3	-	8/18/24/24	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	477	PTG	C7-C8	3.37	1.53	1.43
2	A	1	GSH	CA2-N2	2.90	1.52	1.45
3	A	477	PTG	C13-C14	2.12	1.37	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	GSH	CB2-CA2-N2	-5.88	102.89	111.28
2	A	1	GSH	CB1-CG1-CD1	-3.51	105.19	113.04
2	A	1	GSH	OE1-CD1-CG1	-3.27	116.03	122.02
2	A	1	GSH	CG1-CD1-N2	3.19	121.36	115.83
2	A	1	GSH	C2-CA2-N2	2.47	117.87	111.16
3	A	477	PTG	C14-C15-C10	-2.25	97.40	100.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

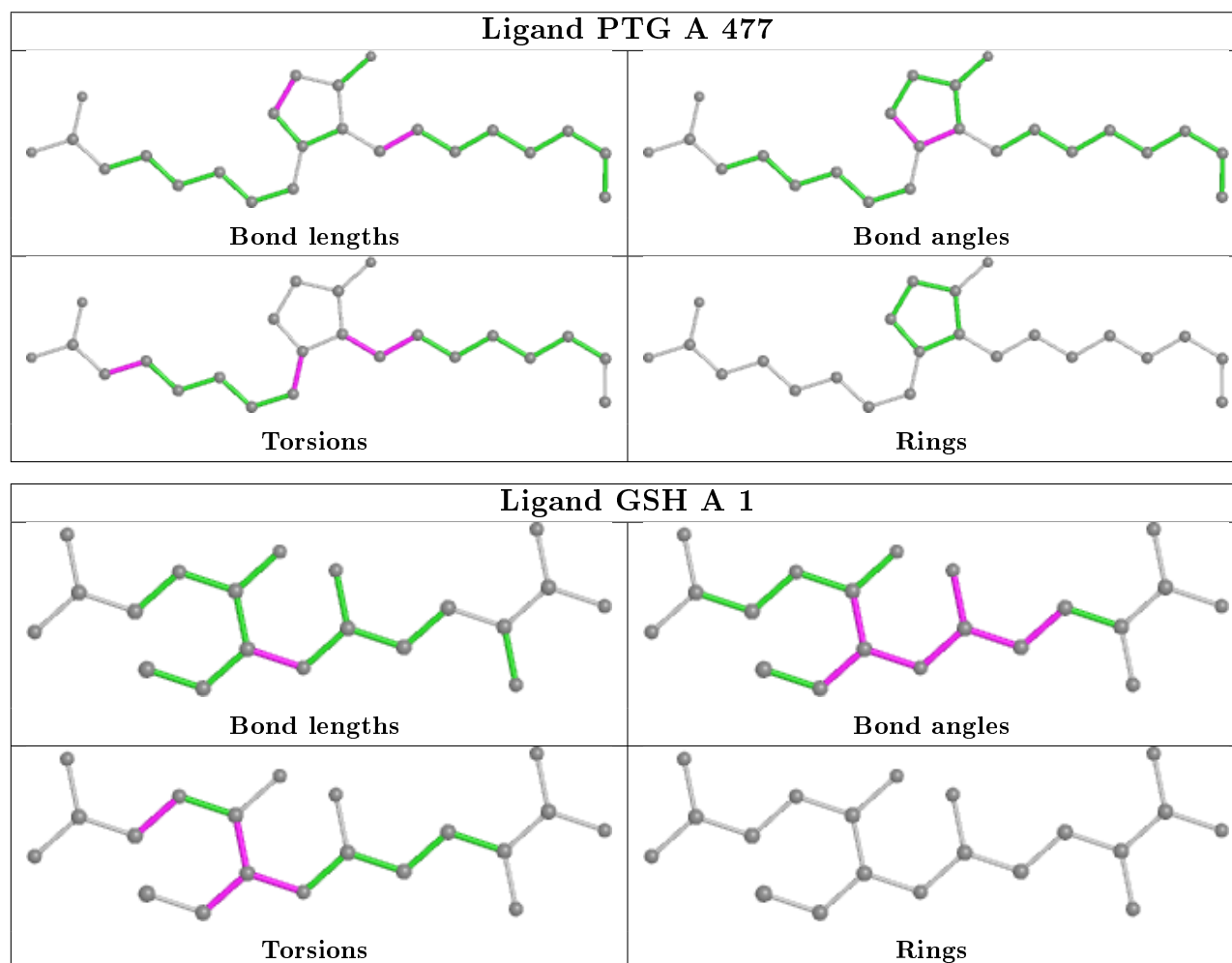
Mol	Chain	Res	Type	Atoms
3	A	477	PTG	C6-C7-C8-C10
3	A	477	PTG	C11-C10-C8-C7
3	A	477	PTG	C15-C10-C8-C7
3	A	477	PTG	C19-C20-C21-C22
2	A	1	GSH	N2-CA2-CB2-SG2
2	A	1	GSH	C2-CA2-CB2-SG2
2	A	1	GSH	C2-CA2-N2-CD1
2	A	1	GSH	O2-C2-CA2-CB2
2	A	1	GSH	N3-C2-CA2-CB2
2	A	1	GSH	O2-C2-CA2-N2
2	A	1	GSH	N3-C2-CA2-N2
2	A	1	GSH	C3-CA3-N3-C2
3	A	477	PTG	C14-C15-C16-C17

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	477	PTG	11	0
2	A	1	GSH	5	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	274/286 (95%)	0.53	15 (5%) 25 27	27, 44, 68, 76	0
1	B	263/286 (91%)	0.82	32 (12%) 4 3	30, 46, 72, 78	0
All	All	537/572 (93%)	0.67	47 (8%) 10 11	27, 45, 71, 78	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	242	THR	7.9
1	B	241	THR	7.5
1	B	363	PHE	5.8
1	A	264	PHE	5.2
1	B	274	SER	5.1
1	B	456	ILE	4.5
1	B	271	GLN	4.4
1	A	270	LEU	4.3
1	A	266	HIS	4.2
1	A	268	THR	4.2
1	B	275	LYS	4.0
1	B	273	GLN	3.7
1	B	264	PHE	3.4
1	B	256	MET	3.4
1	B	240	LYS	3.3
1	A	465	LEU	2.9
1	A	356	LEU	2.8
1	B	243	ASP	2.8
1	B	360	PHE	2.8
1	B	293	VAL	2.7
1	A	299	TYR	2.6
1	B	244	LYS	2.6
1	B	272	GLU	2.6
1	A	240	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	473	TYR	2.5
1	B	276	GLU	2.5
1	A	277	VAL	2.4
1	B	472	ILE	2.4
1	B	352	PHE	2.4
1	B	455	VAL	2.4
1	B	265	LYS	2.3
1	A	267	ILE	2.3
1	B	358	LYS	2.3
1	B	357	ARG	2.3
1	B	361	GLY	2.3
1	B	245	SER	2.3
1	A	262	ILE	2.2
1	A	252	MET	2.2
1	A	269	PRO	2.2
1	A	287	PHE	2.2
1	B	355	SER	2.1
1	B	311	LEU	2.1
1	B	318	LEU	2.1
1	A	261	LYS	2.1
1	B	322	VAL	2.1
1	B	252	MET	2.0
1	B	297	THR	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 carbohydrates 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, 95<sup>th</sup> 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.

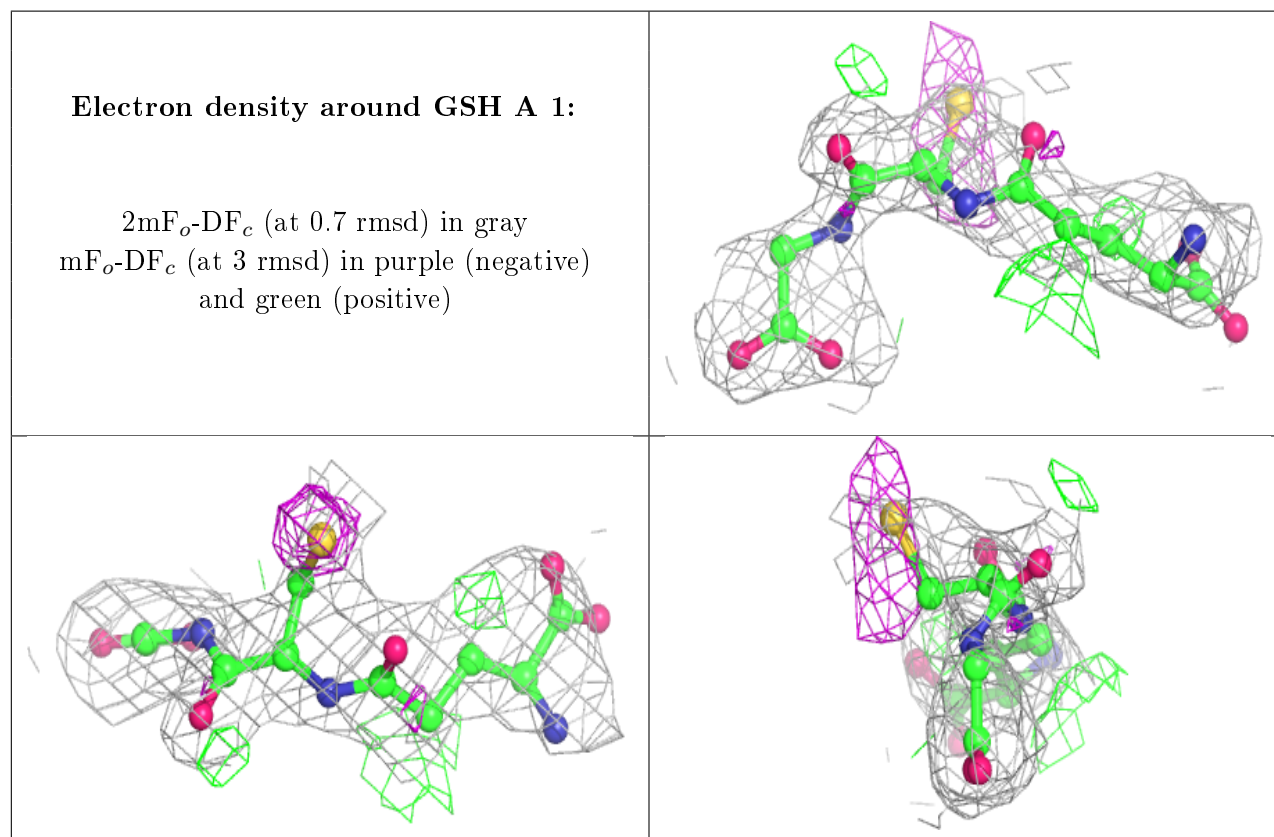
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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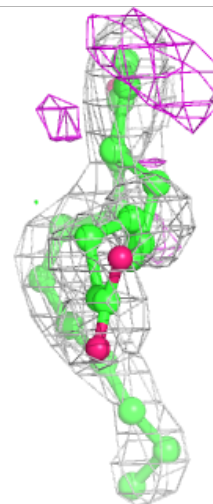
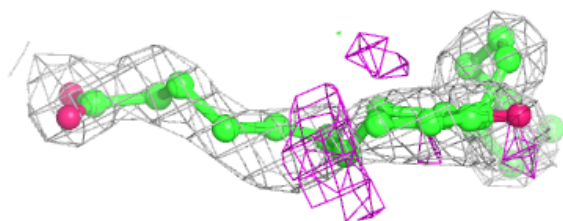
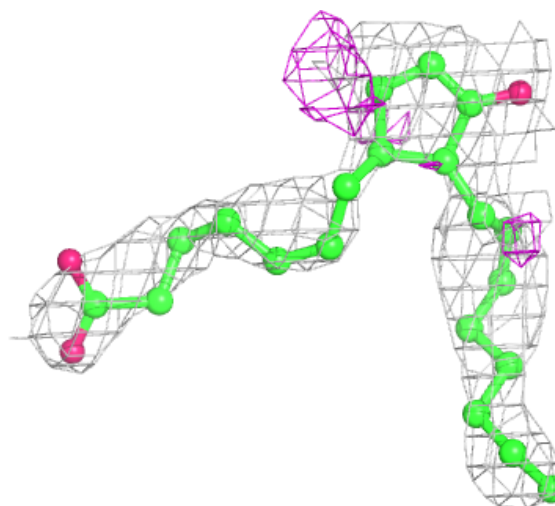
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GSH	A	1	20/20	0.50	0.34	62,72,77,78	0
3	PTG	A	477	23/23	0.76	0.34	53,66,68,69	0

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 PTG A 477:**

$2mF_o-DF_c$  (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.