



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 10:38 pm BST

PDB ID : 3AN3  
Title : Human PPAR gamma ligand binding domain in complex with a gamma selective agonist MO3S  
Authors : Oyama, T.; Ohashi, M.; Waku, T.; Miyachi, H.; Morikawa, K.  
Deposited on : 2010-08-30  
Resolution : 2.30 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

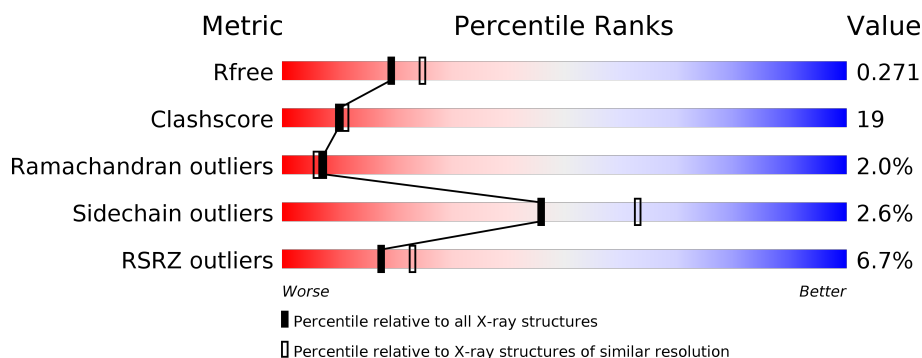
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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>4%</div> <div> <div></div> <div>61%</div> <div>28%</div> <div>• 8%</div> </div> </div>
1	B	286	<div> <div>8%</div> <div> <div></div> <div>63%</div> <div>24%</div> <div>• 10%</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
2	M7S	A	1	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4328 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.

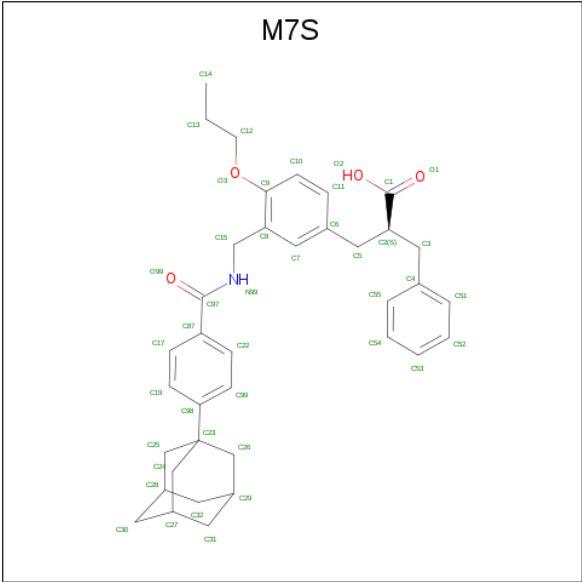
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2102	1354	343	395	10			
1	B	256	Total	C	N	O	S	0	0	0
			2052	1328	336	378	10			

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 (2S)-2-benzyl-3-(4-propoxy-3-({4-[(3S,5S,7S)-tricyclo[3.3.1.1<sup>3,7</sup>]dec-1-yl]phenyl}carbonyl)amino)methyl}phenyl)propanoic acid (three-letter code: M7S) (formula: C<sub>37</sub>H<sub>43</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	37	1	4		

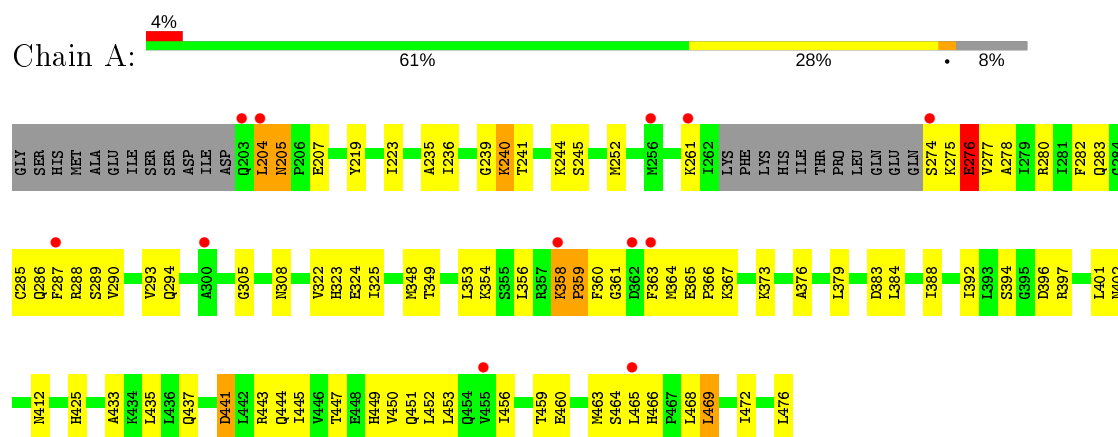
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	72	Total	O	0	0
			72	72		
3	B	60	Total	O	0	0
			60	60		

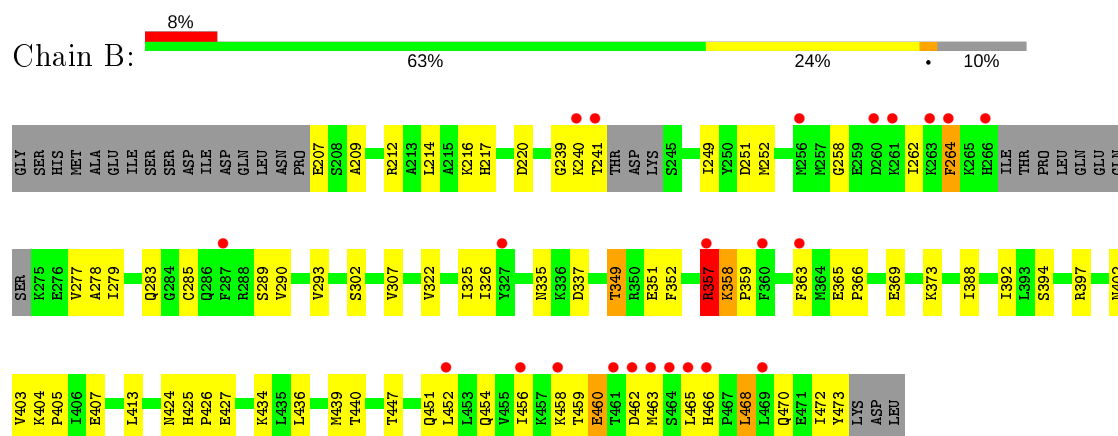
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	93.19 Å   61.06 Å   118.62 Å 90.00°   102.82°   90.00°	Depositor
Resolution (Å)	29.52 – 2.30 45.90 – 2.30	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.52-2.30) 94.6 (45.90-2.30)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.74 (at 2.29 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.227   ,   0.278 0.218   ,   0.271	Depositor DCC
$R_{free}$ test set	1418 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4328	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 5.39% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M7S

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	0.36	0/2136	0.56	0/2877
1	B	0.36	0/2086	0.56	0/2807
All	All	0.36	0/4222	0.56	0/5684

There are no bond length outliers.

There are no bond angle outliers.

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	2102	0	2163	90	0
1	B	2052	0	2112	78	0
2	A	42	0	42	10	0
3	A	72	0	0	9	0
3	B	60	0	0	2	0
All	All	4328	0	4317	162	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 19.

All (162) 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	1.29	0.96
1:B:358:LYS:HB3	1:B:359:PRO:HD2	1.51	0.92
1:B:459:THR:HG22	1:B:460:GLU:H	1.33	0.91
1:A:205:ASN:HD22	1:A:207:GLU:HB2	1.35	0.90
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.00	0.90
1:B:325:ILE:HG23	1:B:388:ILE:HD12	1.55	0.89
1:A:240:LYS:HD3	1:A:241:THR:HG23	1.56	0.87
1:B:357:ARG:HG2	1:B:358:LYS:HG3	1.56	0.86
1:A:205:ASN:ND2	1:A:207:GLU:HB2	1.90	0.86
1:A:235:ALA:HB1	1:A:240:LYS:HD2	1.56	0.86
1:A:469:LEU:HD23	2:A:1:M7S:H54	1.56	0.85
1:A:241:THR:HG21	1:A:244:LYS:HD2	1.60	0.82
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.61	0.81
1:B:466:HIS:HD2	1:B:468:LEU:H	1.32	0.76
1:B:466:HIS:CD2	1:B:468:LEU:H	2.05	0.74
1:A:277:VAL:HG13	1:A:278:ALA:H	1.53	0.73
1:B:322:VAL:O	1:B:326:ILE:HG12	1.91	0.70
1:A:277:VAL:HG13	1:A:278:ALA:N	2.07	0.69
1:A:288:ARG:HG2	2:A:1:M7S:H15	1.75	0.69
1:A:236:ILE:HG12	1:A:244:LYS:HB3	1.76	0.68
1:B:452:LEU:O	1:B:456:ILE:HG12	1.95	0.67
1:A:241:THR:HG21	1:A:244:LYS:CD	2.26	0.65
1:B:277:VAL:HG23	1:B:278:ALA:H	1.62	0.64
1:B:459:THR:HG22	1:B:460:GLU:N	2.10	0.64
1:A:364:MET:SD	2:A:1:M7S:H10	2.39	0.63
1:B:357:ARG:HG2	1:B:358:LYS:N	2.13	0.63
1:B:454:GLN:HB2	1:B:458:LYS:HZ3	1.64	0.62
1:B:465:LEU:H	1:B:470:GLN:HE21	1.48	0.61
1:B:307:VAL:HG22	3:B:1067:HOH:O	2.01	0.61
1:A:441:ASP:O	1:A:445:ILE:HG12	2.00	0.61
1:B:466:HIS:CD2	1:B:468:LEU:HB2	2.35	0.60
1:A:235:ALA:CB	1:A:240:LYS:HD2	2.31	0.60
1:A:240:LYS:NZ	3:A:1069:HOH:O	2.36	0.59
1:B:277:VAL:HG23	1:B:278:ALA:N	2.18	0.59
1:A:261:LYS:NZ	1:A:261:LYS:HB3	2.17	0.59
1:A:443:ARG:HG3	1:B:440:THR:CG2	2.33	0.58
1:B:349:THR:HG23	3:B:1159:HOH:O	2.03	0.58
1:A:348:MET:SD	2:A:1:M7S:H14	2.43	0.58
1:A:412:ASN:HB3	3:A:1139:HOH:O	2.03	0.57
1:A:285:CYS:SG	2:A:1:M7S:H12A	2.45	0.56
1:B:436:LEU:O	1:B:439:MET:HB2	2.04	0.56
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.88	0.56
1:B:216:LYS:HE3	1:B:220:ASP:OD1	2.05	0.56
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.87	0.56
1:B:357:ARG:NH2	1:B:358:LYS:NZ	2.54	0.56
1:B:358:LYS:CB	1:B:359:PRO:HD2	2.32	0.56
1:A:396:ASP:HB2	1:B:373:LYS:NZ	2.20	0.56
1:B:289:SER:O	1:B:293:VAL:HG23	2.06	0.55
1:B:279:ILE:CD1	1:B:462:ASP:HB3	2.37	0.55
1:B:358:LYS:CB	1:B:359:PRO:CD	2.77	0.55
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.89	0.55
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.89	0.54
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.89	0.54
1:A:354:LYS:HA	1:A:361:GLY:O	2.08	0.54
1:B:466:HIS:HD2	1:B:468:LEU:HB2	1.73	0.54
1:B:468:LEU:O	1:B:472:ILE:HG13	2.07	0.54
1:B:249:ILE:HD12	1:B:249:ILE:N	2.23	0.54
1:B:465:LEU:H	1:B:470:GLN:NE2	2.06	0.54
1:B:402:ASN:O	1:B:405:PRO:HD2	2.08	0.53
1:A:394:SER:O	1:A:397:ARG:HG2	2.09	0.52
1:A:456:ILE:HG21	1:A:463:MET:HE1	1.92	0.52
1:B:290:VAL:HG21	1:B:473:TYR:HD1	1.75	0.51
1:A:349:THR:HB	3:A:1187:HOH:O	2.09	0.51
1:A:465:LEU:N	1:A:465:LEU:HD22	2.25	0.51
1:A:280:ARG:HG2	2:A:1:M7S:H30	1.93	0.51
1:A:276:GLU:O	1:A:280:ARG:HB2	2.10	0.50
1:B:217:HIS:HE1	1:B:302:SER:O	1.94	0.50
1:B:258:GLY:O	1:B:262:ILE:HB	2.12	0.50
1:A:239:GLY:C	1:A:241:THR:H	2.15	0.50
1:B:357:ARG:NE	1:B:358:LYS:HD2	2.26	0.50
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.41	0.50
1:B:279:ILE:O	1:B:283:GLN:HG3	2.11	0.50
1:B:447:THR:O	1:B:451:GLN:HG2	2.12	0.50
1:A:241:THR:OG1	1:A:244:LYS:HB2	2.11	0.50
1:B:403:VAL:HG12	1:B:407:GLU:HG3	1.94	0.49
1:A:364:MET:HB2	3:A:1091:HOH:O	2.11	0.49
1:A:277:VAL:CG1	1:A:278:ALA:N	2.76	0.49
1:A:240:LYS:HD3	1:A:240:LYS:C	2.33	0.49
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.43	0.48
1:A:288:ARG:CG	2:A:1:M7S:H15	2.42	0.48
1:A:277:VAL:CG1	1:A:278:ALA:H	2.23	0.48
1:A:384:LEU:O	1:A:388:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:MET:HG2	3:A:1096:HOH:O	2.13	0.48
1:A:433:ALA:O	1:A:437:GLN:HG3	2.13	0.48
1:A:204:LEU:O	1:A:205:ASN:O	2.32	0.47
1:A:245:SER:HA	3:A:1161:HOH:O	2.14	0.47
1:A:449:HIS:CE1	1:A:453:LEU:HD11	2.49	0.47
1:B:451:GLN:O	1:B:454:GLN:HG2	2.14	0.47
1:B:239:GLY:O	1:B:241:THR:N	2.48	0.47
1:B:459:THR:CG2	1:B:460:GLU:H	2.17	0.47
1:A:358:LYS:N	1:A:358:LYS:HD2	2.29	0.47
1:A:290:VAL:O	1:A:294:GLN:HG3	2.14	0.47
1:A:322:VAL:HG21	1:A:472:ILE:HD13	1.96	0.47
1:A:402:ASN:HB3	3:A:1213:HOH:O	2.15	0.47
1:B:472:ILE:O	1:B:472:ILE:HG22	2.15	0.47
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.50	0.47
1:A:358:LYS:H	1:A:358:LYS:CD	2.28	0.46
1:B:357:ARG:NH2	1:B:358:LYS:CE	2.79	0.46
1:A:236:ILE:HG23	1:A:244:LYS:O	2.15	0.46
1:A:373:LYS:O	1:A:376:ALA:HB3	2.16	0.46
1:B:207:GLU:C	1:B:209:ALA:H	2.18	0.46
1:A:235:ALA:HB1	1:A:240:LYS:CD	2.39	0.46
1:A:396:ASP:HB2	1:B:373:LYS:HZ2	1.81	0.46
1:A:402:ASN:N	1:A:402:ASN:HD22	2.12	0.46
1:A:367:LYS:NZ	1:A:449:HIS:HD2	2.14	0.46
1:A:286:GLN:HG2	2:A:1:M7S:C54	2.46	0.46
1:B:460:GLU:HB3	1:B:463:MET:CG	2.46	0.46
1:A:282:PHE:CZ	2:A:1:M7S:H52	2.51	0.45
1:B:262:ILE:HG21	1:B:264:PHE:CE2	2.50	0.45
1:A:443:ARG:HG3	1:B:440:THR:HG23	1.99	0.45
1:B:357:ARG:CG	1:B:358:LYS:N	2.75	0.45
1:A:356:LEU:HB2	1:A:361:GLY:HA2	1.98	0.45
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.97	0.45
1:A:464:SER:O	1:A:465:LEU:HD13	2.16	0.45
1:A:447:THR:O	1:A:451:GLN:HG3	2.16	0.45
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.99	0.45
1:A:463:MET:HE3	1:A:465:LEU:HD11	1.97	0.45
1:B:357:ARG:HE	1:B:358:LYS:HD2	1.81	0.45
1:A:360:PHE:N	1:A:360:PHE:CD1	2.84	0.44
1:A:261:LYS:HZ2	1:A:261:LYS:HB3	1.82	0.44
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.83	0.44
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.99	0.44
1:A:358:LYS:H	1:A:358:LYS:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:CYS:HG	1:B:363:PHE:HZ	1.65	0.44
1:A:241:THR:HG21	1:A:244:LYS:CG	2.48	0.44
1:A:367:LYS:HZ3	1:A:449:HIS:HD2	1.66	0.44
1:A:365:GLU:HB3	1:A:366:PRO:HD3	2.00	0.43
1:B:207:GLU:O	1:B:207:GLU:HG2	2.18	0.43
1:B:251:ASP:C	1:B:251:ASP:OD1	2.56	0.43
1:B:365:GLU:HB3	1:B:366:PRO:HD3	1.99	0.43
1:B:427:GLU:CD	1:B:427:GLU:H	2.21	0.43
1:A:289:SER:O	1:A:293:VAL:HG23	2.19	0.43
1:A:401:LEU:C	1:A:402:ASN:HD22	2.22	0.43
1:A:452:LEU:O	1:A:456:ILE:HG13	2.19	0.43
1:A:274:SER:OG	1:A:275:LYS:N	2.51	0.42
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.54	0.42
1:A:323:HIS:HD2	3:A:1083:HOH:O	2.01	0.42
1:A:402:ASN:ND2	1:A:402:ASN:N	2.68	0.42
1:A:240:LYS:O	1:A:240:LYS:HD3	2.19	0.42
1:A:324:GLU:OE1	1:A:443:ARG:HD3	2.19	0.42
1:B:335:ASN:OD1	1:B:337:ASP:N	2.38	0.41
3:A:1188:HOH:O	1:B:434:LYS:HE2	2.20	0.41
1:B:468:LEU:HD12	1:B:468:LEU:HA	1.76	0.41
1:A:459:THR:HG22	1:A:460:GLU:OE1	2.21	0.41
1:B:349:THR:HG23	1:B:351:GLU:H	1.85	0.41
1:A:443:ARG:CZ	1:B:440:THR:HG21	2.51	0.41
1:A:450:VAL:HG21	1:A:476:LEU:HD23	2.03	0.41
1:A:453:LEU:HD21	2:A:1:M7S:H52	2.03	0.41
1:B:252:MET:SD	1:B:277:VAL:HG11	2.61	0.41
1:B:425:HIS:N	1:B:426:PRO:HD3	2.36	0.41
1:B:465:LEU:HB2	1:B:470:GLN:HG2	2.02	0.41
1:B:460:GLU:HB3	1:B:463:MET:HG2	2.03	0.41
1:B:394:SER:O	1:B:397:ARG:HG2	2.21	0.41
1:B:212:ARG:NE	1:B:212:ARG:HA	2.36	0.40
1:B:335:ASN:C	1:B:335:ASN:OD1	2.60	0.40
1:B:459:THR:O	1:B:460:GLU:HB2	2.22	0.40
1:A:348:MET:SD	1:A:353:LEU:HD21	2.61	0.40
1:A:363:PHE:CE1	1:A:364:MET:HG2	2.56	0.40
1:A:396:ASP:HB2	1:B:373:LYS:HZ1	1.86	0.40
1:B:357:ARG:HH11	1:B:357:ARG:HG3	1.86	0.40
1:B:365:GLU:O	1:B:369:GLU:HG3	2.22	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	259/286 (91%)	245 (95%)	9 (4%)	5 (2%)	8	7
1	B	250/286 (87%)	236 (94%)	9 (4%)	5 (2%)	7	6
All	All	509/572 (89%)	481 (94%)	18 (4%)	10 (2%)	7	6

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	B	240	LYS
1	B	358	LYS
1	B	460	GLU
1	A	204	LEU
1	A	276	GLU
1	B	264	PHE
1	A	359	PRO
1	B	357	ARG
1	A	358	LYS

### 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	236/257 (92%)	228 (97%)	8 (3%)	37	51
1	B	228/257 (89%)	224 (98%)	4 (2%)	59	75
All	All	464/514 (90%)	452 (97%)	12 (3%)	46	63

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	LYS
1	A	276	GLU
1	A	283	GLN
1	A	287	PHE
1	A	441	ASP
1	A	444	GLN
1	A	468	LEU
1	A	469	LEU
1	B	349	THR
1	B	357	ARG
1	B	424	ASN
1	B	468	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	205	ASN
1	A	253	ASN
1	A	294	GLN
1	A	308	ASN
1	A	312	ASN
1	A	323	HIS
1	A	375	ASN
1	A	402	ASN
1	A	425	HIS
1	A	430	GLN
1	A	444	GLN
1	A	449	HIS
1	B	217	HIS
1	B	253	ASN
1	B	283	GLN
1	B	312	ASN
1	B	424	ASN
1	B	430	GLN
1	B	454	GLN
1	B	466	HIS
1	B	470	GLN

### 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 ⓘ

1 ligand is 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	M7S	A	1	-	44,47,47	3.34	32 (72%)	64,67,67	1.24	7 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M7S	A	1	-	-	4/27/58/58	0/7/6/6

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	M7S	C7-C8	7.07	1.51	1.39
2	A	1	M7S	C19-C98	6.47	1.49	1.39
2	A	1	M7S	C7-C6	6.23	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	M7S	C99-C98	5.86	1.48	1.39
2	A	1	M7S	C17-C87	5.06	1.48	1.39
2	A	1	M7S	C19-C17	4.75	1.47	1.38
2	A	1	M7S	C26-C23	4.68	1.61	1.54
2	A	1	M7S	C22-C87	4.65	1.47	1.39
2	A	1	M7S	C99-C22	4.14	1.46	1.38
2	A	1	M7S	C55-C4	4.12	1.47	1.38
2	A	1	M7S	C87-C97	-4.07	1.41	1.50
2	A	1	M7S	C9-C8	3.79	1.46	1.40
2	A	1	M7S	C25-C23	3.71	1.60	1.54
2	A	1	M7S	C24-C23	3.61	1.59	1.54
2	A	1	M7S	C97-N99	3.60	1.41	1.33
2	A	1	M7S	C54-C55	3.23	1.45	1.38
2	A	1	M7S	C10-C9	3.11	1.46	1.39
2	A	1	M7S	C3-C2	3.02	1.58	1.54
2	A	1	M7S	C11-C6	3.01	1.45	1.38
2	A	1	M7S	C54-C53	2.80	1.45	1.38
2	A	1	M7S	C23-C98	2.80	1.58	1.53
2	A	1	M7S	C11-C10	2.60	1.43	1.38
2	A	1	M7S	C52-C51	2.53	1.44	1.38
2	A	1	M7S	C32-C29	2.33	1.58	1.52
2	A	1	M7S	C31-C29	2.32	1.58	1.52
2	A	1	M7S	C30-C28	2.25	1.58	1.52
2	A	1	M7S	C53-C52	2.20	1.43	1.38
2	A	1	M7S	C30-C27	2.19	1.58	1.52
2	A	1	M7S	C5-C2	2.13	1.57	1.54
2	A	1	M7S	C51-C4	2.07	1.43	1.38
2	A	1	M7S	O3-C9	2.05	1.41	1.37
2	A	1	M7S	C3-C4	2.02	1.56	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	M7S	C6-C5-C2	5.72	121.20	113.81
2	A	1	M7S	O3-C9-C8	3.16	119.91	115.78
2	A	1	M7S	C5-C2-C1	-2.77	105.09	111.09
2	A	1	M7S	C4-C3-C2	2.71	117.31	113.81
2	A	1	M7S	C5-C6-C7	2.38	124.51	120.44
2	A	1	M7S	C5-C6-C11	-2.23	116.48	120.91
2	A	1	M7S	C12-O3-C9	-2.21	112.28	117.69

There are no chirality outliers.



All (4) torsion outliers are listed below:

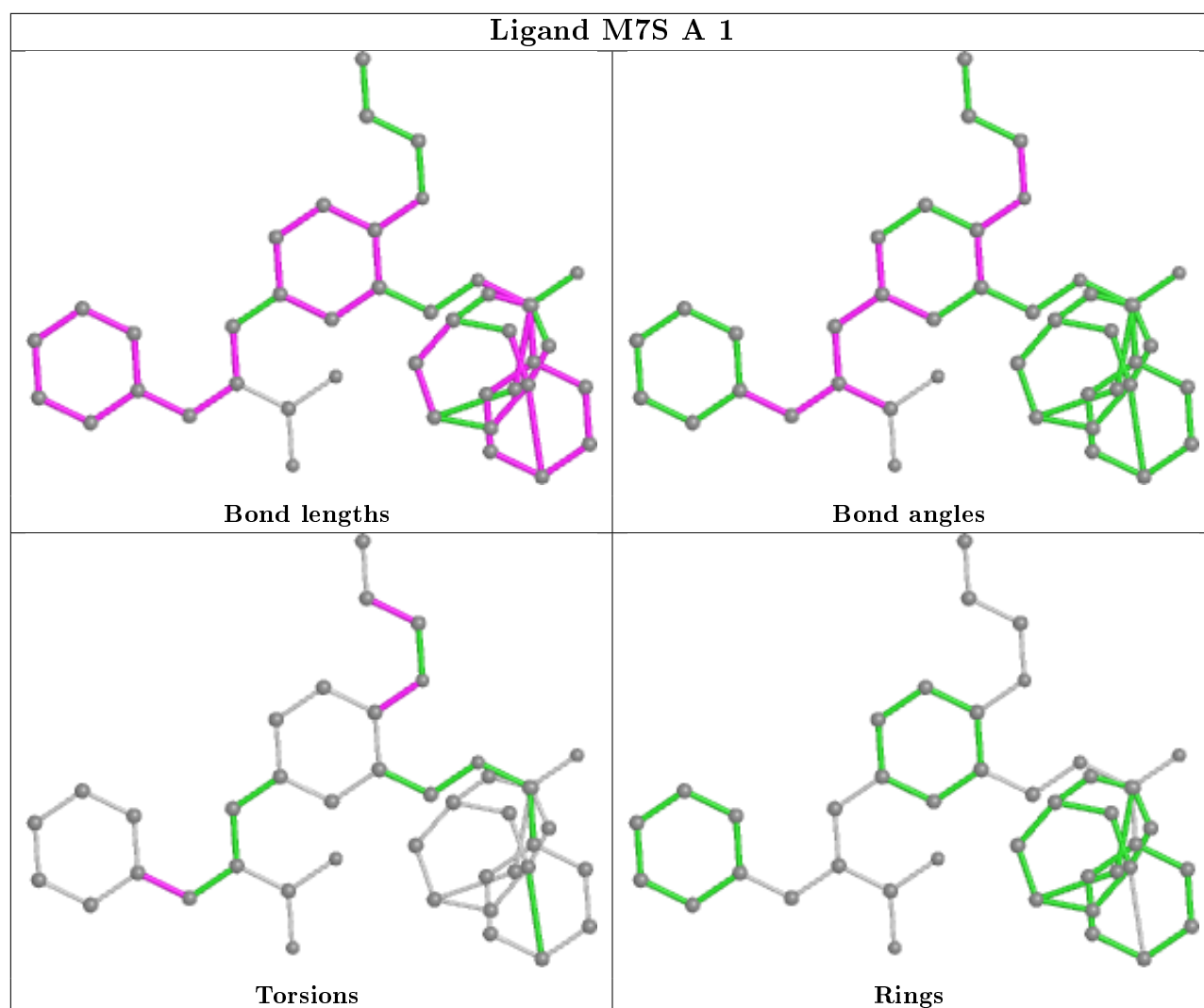
Mol	Chain	Res	Type	Atoms
2	A	1	M7S	O3-C12-C13-C14
2	A	1	M7S	C2-C3-C4-C55
2	A	1	M7S	C2-C3-C4-C51
2	A	1	M7S	C10-C9-O3-C12

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	M7S	10	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, 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	263/286 (91%)	0.29	12 (4%) 32 39	27, 45, 64, 73	0
1	B	256/286 (89%)	0.50	23 (8%) 9 12	26, 46, 68, 73	0
All	All	519/572 (90%)	0.39	35 (6%) 17 23	26, 45, 67, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	464	SER	5.8
1	B	241	THR	5.0
1	A	204	LEU	4.5
1	B	264	PHE	4.2
1	B	465	LEU	4.2
1	B	240	LYS	4.1
1	A	274	SER	4.0
1	B	462	ASP	3.9
1	B	456	ILE	3.8
1	B	458	LYS	3.6
1	A	363	PHE	3.5
1	B	266	HIS	3.2
1	A	203	GLN	3.1
1	B	261	LYS	3.1
1	B	363	PHE	3.0
1	B	287	PHE	2.9
1	B	461	THR	2.8
1	A	465	LEU	2.6
1	B	263	LYS	2.6
1	B	466	HIS	2.5
1	A	287	PHE	2.5
1	B	463	MET	2.5
1	B	357	ARG	2.4
1	A	261	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	260	ASP	2.4
1	B	469	LEU	2.4
1	A	256	MET	2.3
1	A	362	ASP	2.2
1	A	300	ALA	2.2
1	B	256	MET	2.2
1	B	452	LEU	2.1
1	A	455	VAL	2.1
1	B	327	TYR	2.1
1	A	358	LYS	2.1
1	B	360	PHE	2.0

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

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

## 6.3 Carbohydrates ⓘ

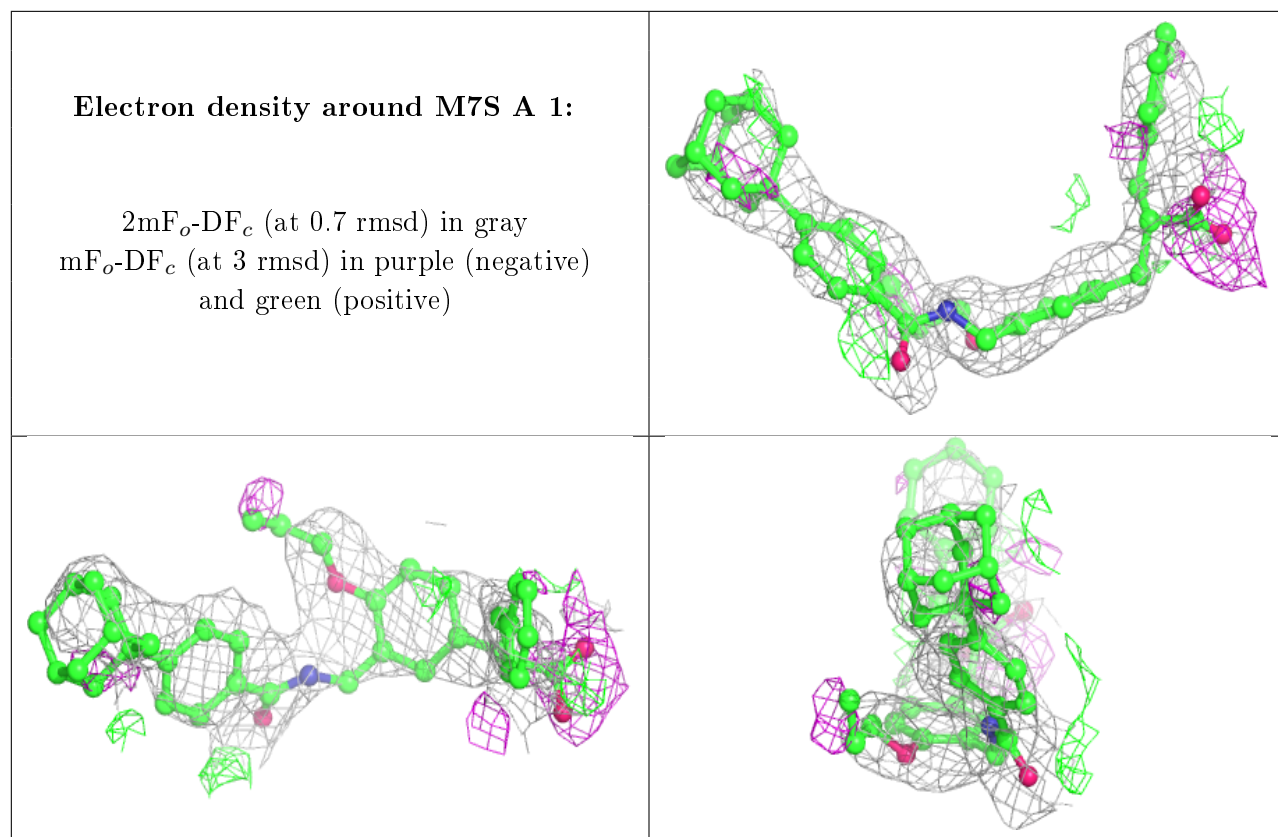
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	M7S	A	1	42/42	0.72	0.47	66,69,72,75	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 [i](#)

There are no such residues in this entry.