



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 03:00 pm GMT

PDB ID : 1Y0S  
Title : Crystal structure of PPAR delta complexed with GW2331  
Authors : Takada, I.; Yu, R.T.; Xu, H.E.; Xu, R.X.; Lambert, M.H.; Montana, V.G.;  
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Deposited on : 2004-11-16  
Resolution : 2.65 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

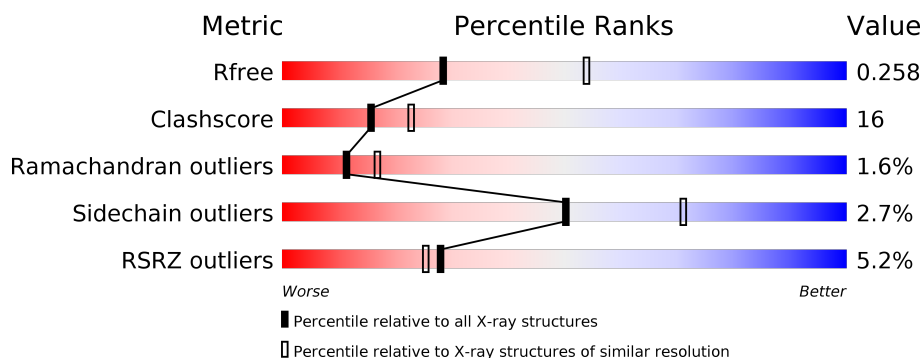
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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))
$R_{free}$	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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. 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	272	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>• •</div> </div> </div>
1	B	272	<div> <div>6%</div> <div> <div></div> <div>61%</div> <div>33%</div> <div>• 5%</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
4	B7G	A	483	X	-	-	X
4	B7G	B	480	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4452 atoms, of which 70 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.

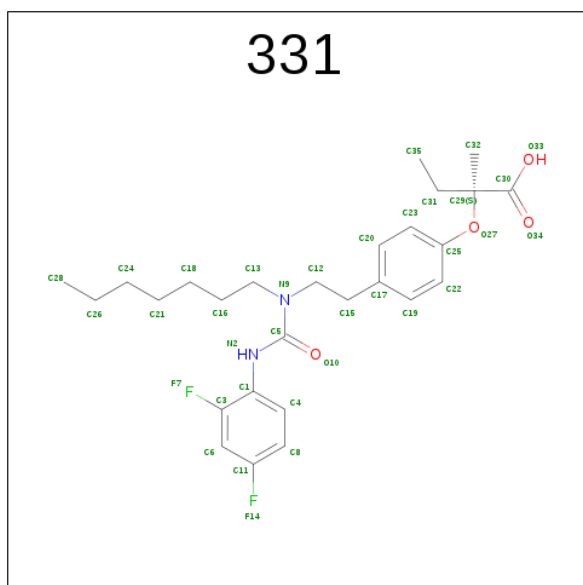
- Molecule 1 is a protein called Peroxisome proliferator activated receptor delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2069	1341	347	372	9			
1	B	258	Total	C	N	O	S	0	0	0
			2032	1316	340	366	10			

- Molecule 2 is IODIDE ION (three-letter code: IOD) (formula: I).

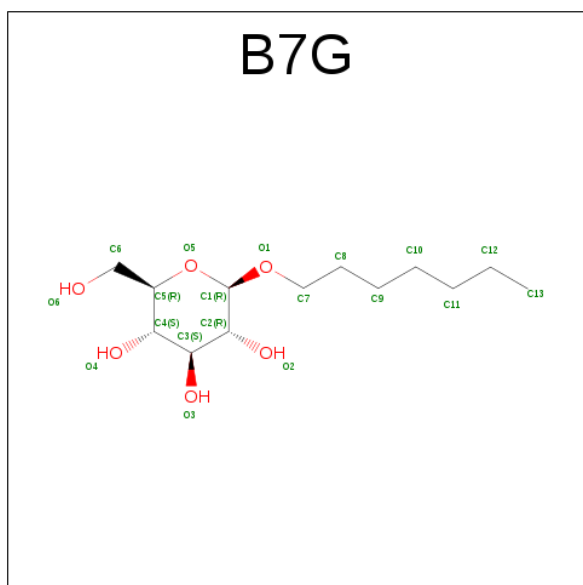
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	I	0	0
			4	4		
2	A	7	Total	I	0	0
			7	7		

- Molecule 3 is (2S)-2-(4-[2-(3-[2,4-DIFLUOROPHENYL]-1-HEPTYLUREIDO)ETHYL]PHENOXY)-2-METHYLBUTYRIC ACID (three-letter code: 331) (formula: C<sub>27</sub>H<sub>36</sub>F<sub>2</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	0	0
			70	27	2	35	2	4		
3	B	1	Total	C	F	H	N	O	0	0
			70	27	2	35	2	4		

- Molecule 4 is HEPTYL-BETA-D-GLUCOPYRANOSIDE (three-letter code: B7G) (formula:  $C_{13}H_{26}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	13	6		
4	B	1	Total	C	O	0	0
			19	13	6		

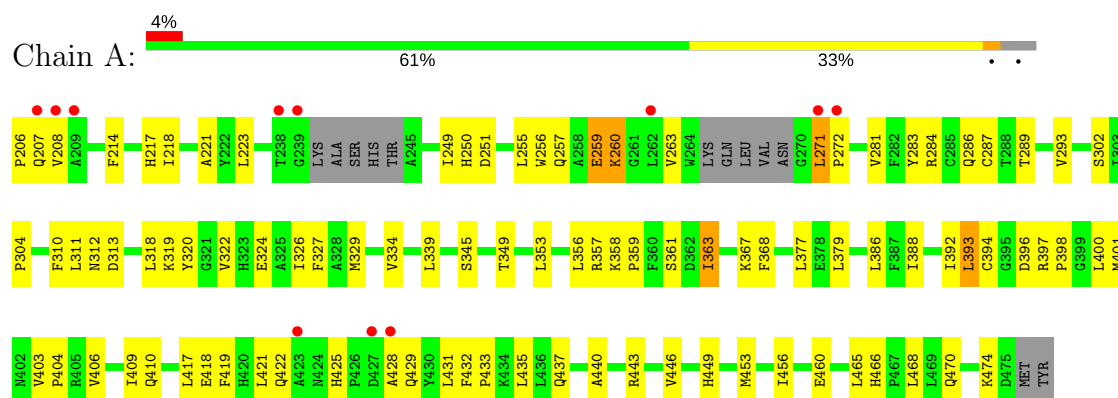
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	78	Total	O	0	0
			78	78		

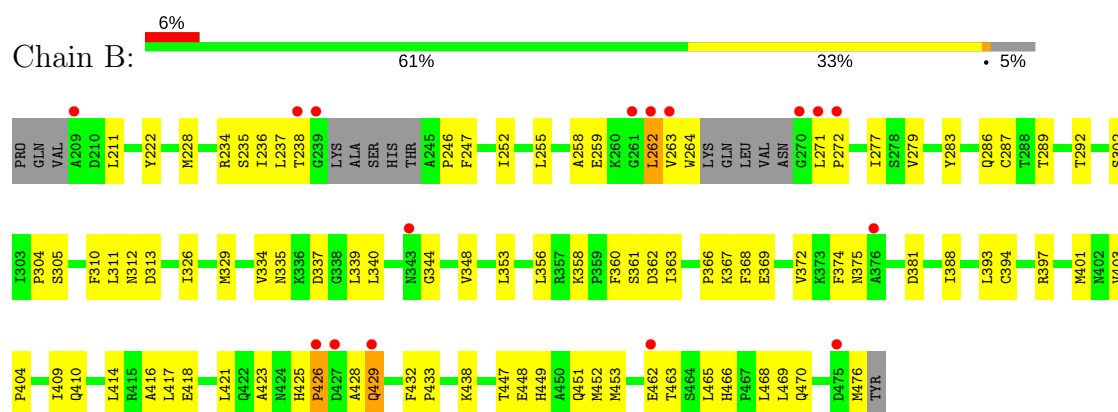
### 3 Residue-property plots

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 delta



- Molecule 1: Peroxisome proliferator activated receptor delta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.36Å 94.52Å 96.49Å 90.00° 97.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.65 19.76 – 2.64	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-2.65) 94.4 (19.76-2.64)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.63Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.210 , 0.261 0.207 , 0.258	Depositor DCC
$R_{free}$ test set	1135 reflections (6.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.5	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 59.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4452	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.10% 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: IOD, 331, B7G

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	0.59	0/2114	0.61	0/2862
1	B	0.57	0/2075	0.59	0/2811
All	All	0.58	0/4189	0.60	0/5673

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	2069	0	2079	65	0
1	B	2032	0	2024	73	0
2	A	7	0	0	0	0
2	B	4	0	0	1	0
3	A	35	35	35	6	0
3	B	35	35	35	6	0
4	A	19	0	19	0	0
4	B	19	0	19	0	0
5	A	84	0	0	2	0
5	B	78	0	0	5	0
All	All	4382	70	4211	138	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 16.

All (138) 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:286:GLN:HA	3:B:479:331:H69	1.50	0.91
1:A:286:GLN:HA	3:A:482:331:H69	1.53	0.88
1:B:432:PHE:HB3	1:B:433:PRO:HD3	1.64	0.79
1:B:258:ALA:HB1	1:B:263:VAL:HG22	1.68	0.75
1:A:356:LEU:O	1:A:361:SER:HB3	1.86	0.75
1:A:334:VAL:HG22	1:A:339:LEU:HB3	1.74	0.70
1:A:256:TRP:CZ2	1:A:260:LYS:HD2	2.27	0.69
1:A:421:LEU:HD11	1:A:435:LEU:HD12	1.74	0.69
1:B:334:VAL:HG22	1:B:339:LEU:HB3	1.75	0.68
1:B:448:GLU:HA	1:B:451:GLN:HG3	1.75	0.67
1:A:319:LYS:HE3	1:A:320:TYR:CZ	2.31	0.66
1:B:463:THR:HG23	5:B:57:HOH:O	1.96	0.64
1:B:234:ARG:O	1:B:238:THR:HG23	1.97	0.64
1:B:289:THR:OG1	3:B:479:331:H70	1.98	0.63
1:B:258:ALA:HA	1:B:262:LEU:CB	2.28	0.63
1:B:292:THR:HG21	1:B:326:ILE:HG12	1.82	0.61
1:A:466:HIS:HD2	1:A:468:LEU:H	1.48	0.61
1:B:277:ILE:HD12	5:B:162:HOH:O	1.98	0.61
1:A:357:ARG:HD2	1:A:358:LYS:O	2.00	0.61
1:B:466:HIS:CD2	1:B:468:LEU:H	2.19	0.61
1:B:366:PRO:HA	1:B:369:GLU:OE1	2.00	0.60
1:A:421:LEU:HD22	1:A:431:LEU:HD23	1.83	0.60
1:A:363:ILE:HD11	3:A:482:331:H54	1.84	0.60
1:B:356:LEU:O	1:B:361:SER:HB3	2.02	0.60
1:B:363:ILE:HD12	1:B:453:MET:HE3	1.82	0.60
1:B:305:SER:HB2	1:B:409:ILE:HD13	1.84	0.59
1:B:449:HIS:O	1:B:453:MET:HG2	2.02	0.58
1:A:388:ILE:O	1:A:392:ILE:HD12	2.03	0.58
1:A:322:VAL:O	1:A:326:ILE:HG13	2.03	0.58
1:B:211:LEU:HD22	1:B:416:ALA:HB2	1.86	0.57
1:B:258:ALA:HB1	1:B:263:VAL:CG2	2.34	0.57
1:B:211:LEU:HD13	1:B:416:ALA:HA	1.85	0.57
1:A:456:ILE:O	1:A:460:GLU:HB2	2.05	0.57
1:B:447:THR:O	1:B:451:GLN:HG2	2.04	0.57
1:A:289:THR:O	1:A:293:VAL:HG23	2.05	0.57
1:A:324:GLU:HG3	1:A:446:VAL:HG21	1.86	0.57
1:B:329:MET:HG2	1:B:388:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:HIS:HD2	1:B:468:LEU:H	1.51	0.56
1:B:462:GLU:HB3	5:B:57:HOH:O	2.05	0.56
1:B:393:LEU:O	1:B:410:GLN:HB2	2.07	0.55
1:B:363:ILE:HD12	1:B:453:MET:CE	2.36	0.55
1:A:313:ASP:OD2	1:A:401:MET:HB3	2.07	0.55
1:A:271:LEU:HD12	1:A:283:TYR:HB3	1.89	0.55
1:A:363:ILE:HD11	3:A:482:331:C22	2.37	0.55
1:A:310:PHE:HB3	1:A:312:ASN:OD1	2.06	0.55
1:B:286:GLN:CA	3:B:479:331:H69	2.30	0.55
1:B:305:SER:HB2	1:B:409:ILE:CD1	2.38	0.54
1:B:465:LEU:HD23	1:B:470:GLN:HG2	1.89	0.54
1:A:363:ILE:HD12	1:A:453:MET:CE	2.37	0.54
1:A:432:PHE:HB3	1:A:433:PRO:CD	2.38	0.54
1:B:358:LYS:HE2	1:B:362:ASP:OD2	2.08	0.54
1:A:363:ILE:HD12	1:A:453:MET:HE1	1.90	0.53
1:A:449:HIS:O	1:A:453:MET:HG2	2.09	0.53
1:B:262:LEU:CB	5:B:13:HOH:O	2.56	0.53
1:A:281:VAL:HG13	3:A:482:331:H57	1.91	0.53
1:A:339:LEU:HD23	1:A:368:PHE:CZ	2.44	0.53
1:A:393:LEU:O	1:A:410:GLN:HB2	2.09	0.52
1:B:263:VAL:HG23	1:B:264:TRP:CD2	2.45	0.51
1:B:310:PHE:HB3	1:B:312:ASN:OD1	2.10	0.51
1:B:237:LEU:HD21	1:B:340:LEU:HG	1.91	0.51
1:A:466:HIS:CD2	1:A:468:LEU:H	2.28	0.50
1:B:428:ALA:O	1:B:429:GLN:O	2.29	0.50
1:A:400:LEU:HD21	1:A:406:VAL:HG21	1.94	0.49
1:B:418:GLU:HB2	1:B:432:PHE:CE1	2.46	0.49
1:B:348:VAL:HG21	3:B:479:331:H61	1.93	0.49
1:A:394:CYS:HB2	5:A:63:HOH:O	2.13	0.49
1:A:289:THR:HA	5:A:155:HOH:O	2.12	0.49
1:B:252:ILE:HD11	1:B:277:ILE:HD13	1.93	0.49
1:B:452:MET:HB2	1:B:453:MET:HE2	1.94	0.49
1:A:466:HIS:HD2	1:A:468:LEU:N	2.11	0.48
1:B:292:THR:CG2	1:B:326:ILE:HG12	2.41	0.48
1:B:360:PHE:O	1:B:363:ILE:HG22	2.14	0.48
1:B:368:PHE:O	1:B:372:VAL:HG23	2.13	0.48
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.95	0.48
1:A:418:GLU:HB2	1:A:432:PHE:CE1	2.49	0.47
1:B:466:HIS:HD2	1:B:468:LEU:N	2.12	0.47
1:B:363:ILE:HD11	3:B:479:331:H54	1.96	0.47
1:A:403:VAL:HB	1:A:404:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:PHE:CZ	1:A:367:LYS:HE2	2.51	0.46
1:B:271:LEU:HD22	1:B:287:CYS:SG	2.56	0.46
1:A:263:VAL:HG13	1:A:345:SER:HB3	1.98	0.46
1:B:403:VAL:HB	1:B:404:PRO:HD3	1.98	0.46
1:B:228:MET:HE1	1:B:236:ILE:HD12	1.98	0.46
1:B:246:PRO:HB3	1:B:344:GLY:O	2.16	0.46
1:B:263:VAL:HG23	1:B:264:TRP:N	2.31	0.46
1:A:214:PHE:CE1	1:A:218:ILE:HD11	2.51	0.46
1:A:250:HIS:CE1	1:A:251:ASP:OD2	2.69	0.45
1:B:367:LYS:N	1:B:367:LYS:HD2	2.31	0.45
1:A:465:LEU:HD23	1:A:470:GLN:HG2	1.99	0.45
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.50	0.45
1:A:393:LEU:HD22	1:A:409:ILE:HG21	1.98	0.45
1:A:256:TRP:CE2	1:A:260:LYS:HD2	2.51	0.45
1:B:313:ASP:OD2	1:B:401:MET:HB3	2.17	0.45
1:B:425:HIS:HA	1:B:426:PRO:HD2	1.57	0.45
1:A:272:PRO:HB2	1:A:283:TYR:CE2	2.51	0.44
1:B:255:LEU:O	1:B:259:GLU:HB2	2.17	0.44
1:A:249:ILE:O	1:A:349:THR:HG23	2.17	0.44
1:A:320:TYR:HB3	1:A:397:ARG:HD2	1.99	0.44
1:A:425:HIS:HB3	1:A:428:ALA:HB2	2.00	0.44
1:B:375:ASN:HA	5:B:75:HOH:O	2.17	0.44
1:A:206:PRO:HB2	1:A:207:GLN:H	1.61	0.44
1:A:271:LEU:HD13	1:A:287:CYS:SG	2.58	0.43
1:A:394:CYS:O	1:A:397:ARG:HG2	2.18	0.43
1:B:235:SER:O	1:B:238:THR:OG1	2.36	0.43
1:B:247:PHE:CE2	1:B:258:ALA:HB2	2.53	0.43
1:B:353:LEU:O	1:B:356:LEU:HG	2.18	0.43
1:B:335:ASN:HA	2:B:201:IOD:I	2.88	0.43
1:B:469:LEU:HD13	3:B:479:331:H64	1.99	0.43
1:A:377:LEU:HB2	1:A:379:LEU:HD13	2.01	0.43
1:B:448:GLU:HA	1:B:451:GLN:CG	2.44	0.43
1:A:318:LEU:O	1:A:322:VAL:HG22	2.18	0.43
1:A:329:MET:HG2	1:A:388:ILE:HD11	2.01	0.42
1:A:431:LEU:HA	1:A:431:LEU:HD12	1.69	0.42
1:B:279:VAL:HG12	1:B:283:TYR:CE2	2.54	0.42
1:A:320:TYR:CB	1:A:397:ARG:HD2	2.48	0.42
1:B:263:VAL:CG2	1:B:264:TRP:CE3	3.03	0.42
1:A:208:VAL:HG12	1:A:208:VAL:O	2.20	0.42
1:A:286:GLN:HG2	3:A:482:331:H64	2.01	0.42
1:B:417:LEU:O	1:B:421:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:O	1:A:392:ILE:CD1	2.68	0.42
1:B:335:ASN:OD1	1:B:337:ASP:N	2.51	0.42
1:A:419:PHE:HD2	1:A:422:GLN:OE1	2.02	0.42
1:A:289:THR:OG1	3:A:482:331:H71	2.20	0.42
1:B:360:PHE:HZ	1:B:463:THR:HG21	1.85	0.42
1:A:217:HIS:CE1	1:A:304:PRO:HD3	2.55	0.42
1:B:311:LEU:HD12	1:B:311:LEU:HA	1.83	0.41
1:A:425:HIS:HB3	1:A:428:ALA:CB	2.50	0.41
1:B:394:CYS:O	1:B:397:ARG:HG2	2.20	0.41
1:A:311:LEU:HD12	1:A:311:LEU:HA	1.85	0.41
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.80	0.41
1:B:234:ARG:HD3	1:B:234:ARG:HA	1.59	0.41
1:A:221:ALA:HB1	1:A:302:SER:HB2	2.03	0.41
1:A:437:GLN:O	1:A:440:ALA:HB3	2.20	0.41
1:A:259:GLU:CD	1:A:284:ARG:HH11	2.24	0.41
1:B:302:SER:O	1:B:304:PRO:HD3	2.21	0.40
1:B:363:ILE:HD11	1:B:449:HIS:HE1	1.86	0.40
1:B:414:LEU:HA	1:B:414:LEU:HD23	1.84	0.40
1:B:374:PHE:HD1	1:B:438:LYS:HD2	1.86	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	254/272 (93%)	237 (93%)	14 (6%)	3 (1%)	15	24
1	B	252/272 (93%)	229 (91%)	18 (7%)	5 (2%)	9	13
All	All	506/544 (93%)	466 (92%)	32 (6%)	8 (2%)	11	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	LYS
1	A	429	GLN
1	B	426	PRO
1	B	429	GLN
1	A	259	GLU
1	B	423	ALA
1	B	262	LEU
1	B	272	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	223/240 (93%)	212 (95%)	11 (5%)	29	46
1	B	216/240 (90%)	215 (100%)	1 (0%)	91	96
All	All	439/480 (92%)	427 (97%)	12 (3%)	50	71

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

Mol	Chain	Res	Type
1	A	223	LEU
1	A	255	LEU
1	A	257	GLN
1	A	271	LEU
1	A	353	LEU
1	A	359	PRO
1	A	363	ILE
1	A	393	LEU
1	A	396	ASP
1	A	443	ARG
1	A	474	LYS
1	B	476	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	HIS
1	A	466	HIS
1	B	217	HIS
1	B	250	HIS
1	B	257	GLN
1	B	422	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 ⓘ

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	331	A	482	-	33,36,36	1.17	3 (9%)	39,48,48	1.31	7 (17%)
4	B7G	A	483	-	19,19,19	3.47	4 (21%)	24,24,24	3.03	9 (37%)
3	331	B	479	-	33,36,36	1.15	2 (6%)	39,48,48	1.26	4 (10%)
4	B7G	B	480	-	19,19,19	3.46	5 (26%)	24,24,24	3.15	11 (45%)

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	331	A	482	-	-	0/28/34/34	0/2/2/2
4	B7G	A	483	-	3/3/5/5	0/10/30/30	0/1/1/1
3	331	B	479	-	-	0/28/34/34	0/2/2/2
4	B7G	B	480	-	3/3/5/5	0/10/30/30	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	483	B7G	O2-C2	-8.57	1.23	1.43
4	B	480	B7G	O2-C2	-8.52	1.23	1.43
4	A	483	B7G	O4-C4	-8.44	1.23	1.43
4	B	480	B7G	O4-C4	-8.34	1.23	1.43
4	B	480	B7G	O3-C3	-8.20	1.24	1.43
4	A	483	B7G	O3-C3	-8.13	1.24	1.43
3	A	482	331	C1-N2	-3.28	1.35	1.41
4	B	480	B7G	O6-C6	-2.70	1.31	1.42
4	A	483	B7G	O6-C6	-2.68	1.31	1.42
3	A	482	331	C8-C11	2.19	1.41	1.37
4	B	480	B7G	O1-C1	2.41	1.44	1.40
3	A	482	331	C1-C3	2.51	1.42	1.38
3	B	479	331	C32-C29	2.67	1.56	1.52
3	B	479	331	C6-C3	3.32	1.43	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	479	331	O27-C29-C32	-3.41	103.42	110.21
4	B	480	B7G	O1-C1-C2	-3.20	103.02	108.23
3	A	482	331	C3-C1-N2	-2.64	113.72	118.54
3	A	482	331	C12-C15-C17	-2.59	104.17	112.21
3	B	479	331	C12-C15-C17	-2.28	105.13	112.21
3	A	482	331	C18-C16-C13	-2.08	103.32	113.25
3	A	482	331	F14-C11-C6	-2.02	115.31	118.24
3	A	482	331	C4-C1-C3	2.04	119.13	117.16
4	B	480	B7G	O5-C1-O1	2.11	115.02	110.02
3	A	482	331	C4-C1-N2	2.25	127.15	121.84
3	A	482	331	C19-C22-C25	2.29	122.61	119.74
3	B	479	331	F14-C11-C6	2.33	121.63	118.24
4	A	483	B7G	C4-C3-C2	2.47	115.20	110.84
4	B	480	B7G	C7-O1-C1	2.66	118.43	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	479	331	C1-N2-C5	2.69	132.15	126.06
4	A	483	B7G	C3-C4-C5	2.85	115.23	110.22
4	B	480	B7G	C3-C4-C5	4.27	117.74	110.22
4	A	483	B7G	C1-C2-C3	4.29	117.95	109.98
4	B	480	B7G	O2-C2-C3	4.53	120.22	110.36
4	B	480	B7G	O4-C4-C5	4.54	120.73	109.28
4	A	483	B7G	O3-C3-C4	4.62	120.42	110.36
4	A	483	B7G	O4-C4-C5	4.87	121.55	109.28
4	A	483	B7G	O2-C2-C1	4.88	120.23	110.03
4	B	480	B7G	O2-C2-C1	4.95	120.38	110.03
4	B	480	B7G	C1-C2-C3	5.07	119.39	109.98
4	B	480	B7G	O4-C4-C3	5.13	121.52	110.36
4	A	483	B7G	O2-C2-C3	5.27	121.82	110.36
4	B	480	B7G	O3-C3-C2	5.47	122.27	110.36
4	A	483	B7G	O4-C4-C3	5.91	123.21	110.36
4	B	480	B7G	O3-C3-C4	6.11	123.64	110.36
4	A	483	B7G	O3-C3-C2	6.44	124.38	110.36

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	483	B7G	C4
4	A	483	B7G	C3
4	A	483	B7G	C2
4	B	480	B7G	C4
4	B	480	B7G	C3
4	B	480	B7G	C2

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	482	331	6	0
3	B	479	331	6	0

## 5.7 Other polymers [\(i\)](#)

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	260/272 (95%)	0.01	11 (4%) 37 34	27, 43, 69, 90	0
1	B	258/272 (94%)	0.20	16 (6%) 21 19	28, 49, 77, 92	0
All	All	518/544 (95%)	0.11	27 (5%) 28 25	27, 46, 73, 92	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	VAL	7.2
1	B	239	GLY	6.4
1	B	209	ALA	5.1
1	A	209	ALA	4.0
1	B	262	LEU	4.0
1	A	262	LEU	3.7
1	B	271	LEU	3.7
1	B	270	GLY	3.6
1	A	207	GLN	3.6
1	B	427	ASP	3.5
1	A	239	GLY	3.5
1	B	261	GLY	3.5
1	B	426	PRO	2.8
1	A	238	THR	2.7
1	B	272	PRO	2.6
1	B	343	ASN	2.6
1	A	428	ALA	2.5
1	A	271	LEU	2.4
1	B	475	ASP	2.4
1	A	423	ALA	2.2
1	B	376	ALA	2.2
1	A	272	PRO	2.1
1	B	429	GLN	2.1
1	B	238	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	263	VAL	2.1
1	B	462	GLU	2.0
1	A	427	ASP	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	B7G	A	483	19/19	0.77	0.28	2.24	43,58,62,63	0
4	B7G	B	480	19/19	0.77	0.26	1.71	35,60,62,63	0
3	331	B	479	35/35	0.94	0.18	-0.07	39,46,55,56	0
3	331	A	482	35/35	0.96	0.15	-0.48	29,36,43,48	0
2	IOD	A	479	1/1	0.81	0.15	-0.74	200,200,200,200	0
2	IOD	B	478	1/1	0.85	0.17	-0.83	200,200,200,200	0
2	IOD	B	205	1/1	0.92	0.09	-1.27	106,106,106,106	0
2	IOD	B	204	1/1	0.90	0.08	-1.38	158,158,158,158	0
2	IOD	A	202	1/1	0.97	0.04	-2.13	85,85,85,85	0
2	IOD	A	200	1/1	0.99	0.05	-2.14	64,64,64,64	0
2	IOD	B	201	1/1	0.99	0.05	-3.66	80,80,80,80	0
2	IOD	A	203	1/1	0.89	0.17	-	167,167,167,167	0
2	IOD	A	480	1/1	0.98	0.06	-	91,91,91,91	0
2	IOD	A	481	1/1	0.95	0.05	-	96,96,96,96	0
2	IOD	A	478	1/1	0.72	0.10	-	158,158,158,158	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.