



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:32 pm BST

PDB ID : 3ADV  
Title : Human PPARgamma ligand-binding domain in complex with serotonin  
Authors : Waku, T.; Shiraki, T.; Oyama, T.; Morikawa, K.  
Deposited on : 2010-01-29  
Resolution : 2.27 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  
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

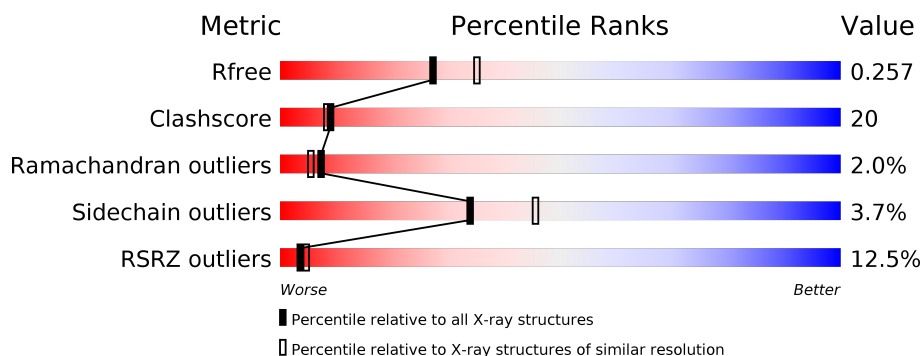
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	287	<div> <div>8%</div> <div>61%</div> <div>27%</div> <div>• 9%</div> </div>
1	B	287	<div> <div>15%</div> <div>60%</div> <div>27%</div> <div>•• 10%</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	SRO	A	3	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4294 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.

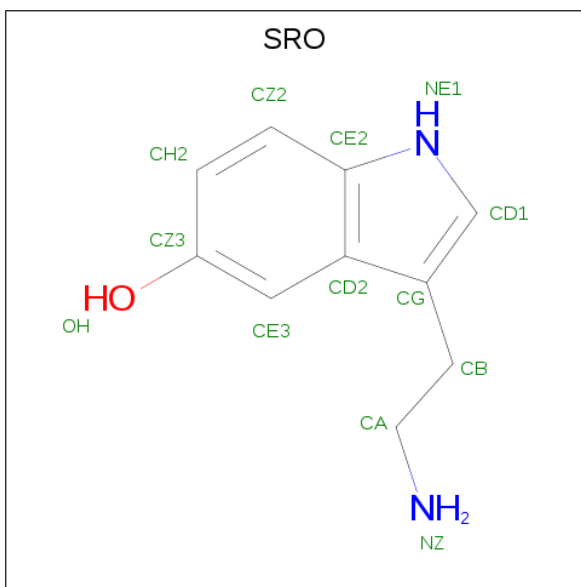
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2083	1343	340	390	10			
1	B	257	Total	C	N	O	S	0	0	0
			2063	1336	338	380	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 SEROTONIN (three-letter code: SRO) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	10	2	1		
2	A	1	Total	C	N	O	0	0
			13	10	2	1		
2	B	1	Total	C	N	O	0	0
			13	10	2	1		

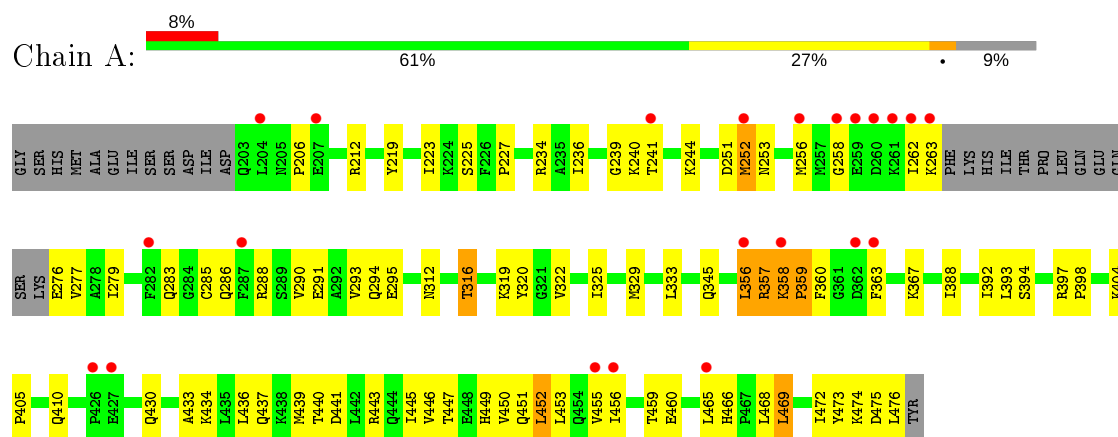
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	49	Total	O	0	0
			49	49		

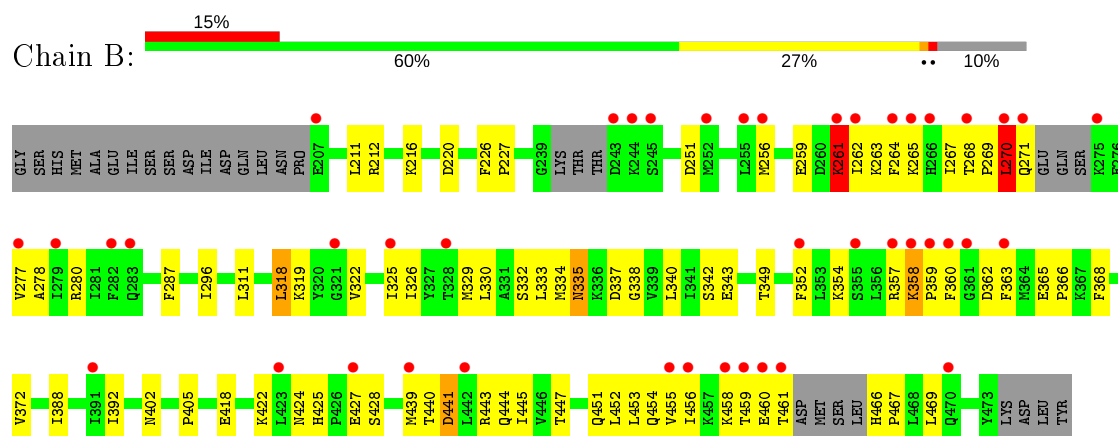
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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, $\alpha$ , $\beta$ , $\gamma$	93.06 Å   61.46 Å   118.47 Å 90.00°   102.89°   90.00°	Depositor
Resolution (Å)	44.60 – 2.27 44.55 – 2.27	Depositor EDS
% Data completeness (in resolution range)	92.1 (44.60-2.27) 93.1 (44.55-2.27)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.80 (at 2.27 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224   ,   0.267 0.215   ,   0.257	Depositor DCC
$R_{free}$ test set	1431 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.2	Xtriage
Anisotropy	0.608	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 51.4	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	0.94	EDS
Total number of atoms	4294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: SRO

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	0/2116	0.58	1/2851 (0.0%)
1	B	0.34	0/2097	0.55	0/2822
All	All	0.35	0/4213	0.57	1/5673 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	PRO	N-CA-CB	5.13	109.46	103.30

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	2083	0	2133	87	0
1	B	2063	0	2126	88	0
2	A	26	0	22	4	0
2	B	13	0	11	0	0
3	A	60	0	0	3	0
3	B	49	0	0	1	0
All	All	4294	0	4292	171	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 20.

All (171) 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:358:LYS:HB3	1:B:359:PRO:HD2	1.19	1.09
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.39	1.01
1:A:252:MET:HE1	1:A:277:VAL:HG21	1.43	0.96
1:B:358:LYS:HB3	1:B:359:PRO:CD	1.94	0.96
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.54	0.89
1:A:329:MET:HB3	2:A:3:SRO:HA2	1.55	0.89
1:B:265:LYS:HG2	1:B:269:PRO:HG3	1.56	0.85
1:B:349:THR:HG23	1:B:352:PHE:H	1.42	0.84
1:B:267:ILE:HG13	1:B:268:THR:N	1.97	0.78
1:B:267:ILE:O	1:B:270:LEU:HG	1.84	0.78
1:A:241:THR:OG1	1:A:244:LYS:HB2	1.86	0.75
1:A:333:LEU:HD21	2:A:3:SRO:HNZ1	1.52	0.74
1:A:459:THR:HG23	1:A:460:GLU:HG2	1.71	0.72
1:A:433:ALA:O	1:A:437:GLN:HG3	1.90	0.70
1:A:291:GLU:HA	1:A:294:GLN:OE1	1.91	0.69
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.74	0.69
1:B:267:ILE:HG13	1:B:268:THR:H	1.54	0.69
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.73	0.69
1:B:335:ASN:HD22	1:B:335:ASN:C	1.94	0.69
1:A:241:THR:HG21	1:A:244:LYS:HD2	1.76	0.67
1:B:261:LYS:HA	1:B:261:LYS:HE3	1.75	0.67
1:B:418:GLU:O	1:B:422:LYS:HG2	1.94	0.67
1:A:227:PRO:HD2	2:A:3:SRO:HNE1	1.60	0.67
1:B:453:LEU:O	1:B:456:ILE:HG22	1.96	0.66
1:B:335:ASN:ND2	1:B:337:ASP:H	1.93	0.66
1:A:293:VAL:HG11	1:A:468:LEU:HD11	1.77	0.65
1:B:263:LYS:C	1:B:265:LYS:H	1.98	0.65
1:A:437:GLN:O	1:A:440:THR:HG22	1.96	0.65
1:B:363:PHE:CE1	1:B:452:LEU:HB3	2.32	0.65
1:A:244:LYS:HE2	3:A:1106:HOH:O	1.96	0.65
1:A:441:ASP:O	1:A:445:ILE:HG12	1.97	0.65
1:B:335:ASN:ND2	1:B:338:GLY:H	1.95	0.65
1:A:239:GLY:C	1:A:241:THR:H	2.01	0.65
1:A:443:ARG:NH1	1:B:444:GLN:HE22	1.94	0.65
1:A:472:ILE:O	1:A:476:LEU:HG	1.98	0.64
1:A:252:MET:CE	1:A:252:MET:HA	2.28	0.64
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.23	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:ARG:O	1:B:447:THR:HG23	1.98	0.63
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.64	0.63
1:A:258:GLY:O	1:A:262:ILE:HG12	1.98	0.62
1:B:451:GLN:HE21	1:B:451:GLN:HA	1.64	0.62
1:B:259:GLU:CD	1:B:280:ARG:HH12	2.04	0.61
1:A:252:MET:CE	1:A:277:VAL:HG21	2.25	0.60
1:A:363:PHE:CD2	1:A:452:LEU:HD13	2.37	0.59
1:A:241:THR:HG21	1:A:244:LYS:CG	2.32	0.59
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.37	0.59
1:A:456:ILE:HA	1:A:459:THR:CG2	2.33	0.59
1:A:447:THR:O	1:A:451:GLN:HG3	2.03	0.58
1:B:451:GLN:O	1:B:454:GLN:HG2	2.03	0.58
1:A:393:LEU:O	1:A:410:GLN:HB2	2.04	0.57
1:B:226:PHE:HE1	1:B:296:ILE:HD13	1.69	0.57
1:A:449:HIS:O	1:A:453:LEU:HD23	2.04	0.57
1:A:252:MET:HE3	1:A:252:MET:HA	1.85	0.57
1:A:236:ILE:HG12	1:A:244:LYS:HB3	1.87	0.57
1:B:357:ARG:NH1	1:B:358:LYS:HD2	2.20	0.57
1:B:267:ILE:HG22	1:B:287:PHE:CB	2.34	0.57
1:B:402:ASN:O	1:B:405:PRO:HD2	2.05	0.56
1:A:452:LEU:O	1:A:456:ILE:HG12	2.06	0.56
1:A:252:MET:O	1:A:256:MET:HG3	2.05	0.56
1:A:263:LYS:HE3	1:A:345:GLN:HE22	1.70	0.56
1:B:363:PHE:CD1	1:B:452:LEU:HD23	2.41	0.56
1:A:356:LEU:O	1:A:357:ARG:HB2	2.06	0.55
1:B:265:LYS:HG2	1:B:269:PRO:CG	2.32	0.55
1:B:466:HIS:HB3	1:B:467:PRO:HD3	1.88	0.55
1:B:270:LEU:HD23	1:B:469:LEU:HD21	1.89	0.55
1:B:460:GLU:HG3	1:B:461:THR:N	2.22	0.55
1:B:226:PHE:CE1	1:B:296:ILE:HD13	2.42	0.55
1:B:440:THR:O	1:B:444:GLN:HG3	2.07	0.55
1:A:456:ILE:HA	1:A:459:THR:HG22	1.88	0.54
1:A:241:THR:HG21	1:A:244:LYS:CD	2.38	0.54
1:A:360:PHE:HA	1:A:363:PHE:HD1	1.73	0.54
1:A:363:PHE:CE2	1:A:452:LEU:HD13	2.43	0.54
1:B:349:THR:HG22	1:B:352:PHE:HB3	1.89	0.54
1:A:443:ARG:HH12	1:B:444:GLN:HE22	1.56	0.54
1:A:473:TYR:HA	1:A:476:LEU:HD12	1.91	0.53
1:B:216:LYS:HE3	1:B:220:ASP:OD1	2.09	0.53
1:A:436:LEU:HD22	1:A:439:MET:HE1	1.89	0.53
1:A:465:LEU:HD12	1:A:466:HIS:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LYS:HB2	1:B:319:LYS:NZ	2.24	0.53
1:A:290:VAL:HG22	1:A:469:LEU:HD13	1.91	0.53
1:A:241:THR:HG21	1:A:244:LYS:HG3	1.90	0.53
1:A:363:PHE:CZ	1:A:452:LEU:HD22	2.44	0.53
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.40	0.52
1:B:451:GLN:NE2	1:B:451:GLN:HA	2.24	0.52
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.44	0.52
1:A:455:VAL:O	1:A:459:THR:HG22	2.09	0.52
1:B:267:ILE:CG1	1:B:268:THR:N	2.71	0.52
1:A:446:VAL:O	1:A:450:VAL:HG23	2.09	0.51
1:B:460:GLU:HG3	1:B:461:THR:H	1.75	0.51
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.24	0.51
1:A:436:LEU:HA	1:A:439:MET:HE2	1.92	0.51
1:A:443:ARG:NH1	1:B:444:GLN:NE2	2.59	0.50
1:A:225:SER:O	1:A:295:GLU:HG2	2.12	0.50
1:A:465:LEU:HD12	1:A:466:HIS:N	2.27	0.50
1:A:430:GLN:O	1:A:434:LYS:HG3	2.12	0.49
1:B:268:THR:OG1	1:B:269:PRO:HD3	2.11	0.49
1:B:349:THR:CG2	1:B:352:PHE:H	2.21	0.49
1:A:241:THR:HG22	3:A:1003:HOH:O	2.11	0.49
1:A:253:ASN:HA	1:A:256:MET:CE	2.42	0.49
1:A:279:ILE:O	1:A:283:GLN:HG2	2.13	0.49
1:B:330:LEU:O	1:B:334:MET:HG3	2.13	0.48
1:A:357:ARG:O	1:A:359:PRO:N	2.47	0.48
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.95	0.48
1:B:427:GLU:HG3	1:B:428:SER:N	2.27	0.48
1:A:363:PHE:CG	1:A:452:LEU:HD13	2.49	0.48
1:A:363:PHE:CE1	1:A:452:LEU:HD22	2.48	0.48
1:A:333:LEU:HD11	2:A:3:SRO:HE3	1.95	0.48
1:B:365:GLU:HB3	1:B:366:PRO:HD3	1.94	0.48
1:B:263:LYS:C	1:B:265:LYS:N	2.66	0.48
1:B:335:ASN:ND2	1:B:338:GLY:N	2.60	0.48
1:B:267:ILE:HG22	1:B:287:PHE:HB3	1.95	0.47
1:B:368:PHE:O	1:B:372:VAL:HG23	2.14	0.47
1:B:441:ASP:O	1:B:445:ILE:HD13	2.14	0.47
1:B:267:ILE:CG1	1:B:268:THR:H	2.24	0.47
1:B:360:PHE:HE2	1:B:459:THR:HG21	1.80	0.47
1:A:363:PHE:O	1:A:367:LYS:NZ	2.47	0.47
1:B:357:ARG:NH1	1:B:358:LYS:CD	2.78	0.47
1:B:269:PRO:O	1:B:271:GLN:N	2.48	0.47
1:B:349:THR:HG22	1:B:352:PHE:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ASN:C	1:B:335:ASN:ND2	2.67	0.46
1:A:263:LYS:HE3	1:A:345:GLN:NE2	2.30	0.46
1:B:259:GLU:HA	1:B:264:PHE:CE1	2.51	0.46
1:B:267:ILE:HG22	1:B:287:PHE:CG	2.51	0.46
1:B:354:LYS:HD3	1:B:365:GLU:OE1	2.15	0.46
1:A:449:HIS:NE2	1:A:453:LEU:HD21	2.30	0.46
1:B:277:VAL:HG23	1:B:278:ALA:H	1.81	0.46
1:B:357:ARG:HH11	1:B:358:LYS:HG3	1.81	0.46
1:B:357:ARG:HD2	1:B:358:LYS:HB2	1.98	0.46
1:B:335:ASN:HD22	1:B:337:ASP:H	1.62	0.46
1:B:335:ASN:ND2	1:B:337:ASP:N	2.63	0.46
1:A:312:ASN:O	1:A:316:THR:HG23	2.15	0.46
1:B:363:PHE:CZ	1:B:452:LEU:HB3	2.50	0.45
1:B:427:GLU:HG3	1:B:428:SER:H	1.81	0.45
1:B:268:THR:N	1:B:269:PRO:CD	2.80	0.45
1:B:277:VAL:HG23	1:B:278:ALA:N	2.31	0.45
1:A:474:LYS:O	1:A:475:ASP:HB2	2.16	0.45
1:B:335:ASN:HD21	1:B:338:GLY:N	2.15	0.45
1:B:277:VAL:HG12	1:B:280:ARG:NH2	2.32	0.44
1:B:322:VAL:O	1:B:326:ILE:HG13	2.17	0.44
1:B:251:ASP:HA	1:B:352:PHE:CD1	2.53	0.44
1:B:454:GLN:HG3	1:B:455:VAL:N	2.33	0.44
1:A:241:THR:CG2	1:A:244:LYS:HD2	2.47	0.44
1:A:276:GLU:HG2	1:A:279:ILE:HG13	2.00	0.44
1:A:404:LYS:N	1:A:405:PRO:HD2	2.33	0.44
1:B:311:LEU:HD22	1:B:311:LEU:N	2.32	0.44
1:A:212:ARG:HA	1:A:212:ARG:HD2	1.80	0.43
1:A:325:ILE:HD13	1:A:388:ILE:HG23	2.00	0.43
1:B:296:ILE:HD12	1:B:325:ILE:HG21	2.01	0.43
1:A:253:ASN:HA	1:A:256:MET:HE2	2.01	0.43
1:B:458:LYS:HG3	3:B:1099:HOH:O	2.19	0.42
1:B:342:SER:C	1:B:343:GLU:HG3	2.39	0.42
1:A:319:LYS:HD3	1:A:320:TYR:CE1	2.54	0.42
1:A:234:ARG:HD2	3:A:1113:HOH:O	2.20	0.42
1:A:234:ARG:HD3	1:A:234:ARG:HA	1.85	0.42
1:A:437:GLN:HG2	1:B:439:MET:CE	2.50	0.42
1:B:318:LEU:HA	1:B:318:LEU:HD12	1.77	0.42
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.46	0.42
1:A:286:GLN:NE2	1:A:466:HIS:H	2.17	0.42
1:B:447:THR:O	1:B:451:GLN:HG2	2.19	0.42
1:A:239:GLY:C	1:A:241:THR:N	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:LYS:HG3	1:B:262:ILE:N	2.35	0.41
1:B:440:THR:HG22	1:B:444:GLN:HE21	1.85	0.41
1:B:335:ASN:HD22	1:B:338:GLY:H	1.69	0.41
1:B:325:ILE:HD13	1:B:388:ILE:HG23	2.02	0.41
1:B:425:HIS:HB3	1:B:428:SER:OG	2.20	0.41
1:A:436:LEU:HD22	1:A:439:MET:CE	2.51	0.41
1:B:212:ARG:HA	1:B:212:ARG:NE	2.37	0.40
1:A:392:ILE:HG22	1:A:393:LEU:HD22	2.02	0.40
1:A:397:ARG:HA	1:A:398:PRO:HD3	1.93	0.40
1:B:329:MET:O	1:B:332:SER:HB2	2.22	0.40
1:A:251:ASP:OD1	1:A:253:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/287 (90%)	243 (94%)	9 (4%)	6 (2%)	6	4
1	B	249/287 (87%)	234 (94%)	11 (4%)	4 (2%)	9	8
All	All	507/574 (88%)	477 (94%)	20 (4%)	10 (2%)	7	5

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	B	270	LEU
1	B	358	LYS
1	A	357	ARG
1	A	240	LYS
1	A	359	PRO
1	A	394	SER

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Mol	Chain	Res	Type
1	B	261	LYS
1	A	356	LEU
1	B	227	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	231/258 (90%)	225 (97%)	6 (3%)	46	60
1	B	230/258 (89%)	219 (95%)	11 (5%)	25	34
All	All	461/516 (89%)	444 (96%)	17 (4%)	34	45

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	252	MET
1	A	285	CYS
1	A	288	ARG
1	A	316	THR
1	A	452	LEU
1	A	469	LEU
1	B	211	LEU
1	B	256	MET
1	B	261	LYS
1	B	270	LEU
1	B	318	LEU
1	B	333	LEU
1	B	335	ASN
1	B	340	LEU
1	B	362	ASP
1	B	424	ASN
1	B	441	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	286	GLN
1	A	308	ASN
1	A	424	ASN
1	A	430	GLN
1	B	217	HIS
1	B	271	GLN
1	B	283	GLN
1	B	308	ASN
1	B	335	ASN
1	B	424	ASN
1	B	430	GLN
1	B	444	GLN
1	B	451	GLN
1	B	454	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 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	SRO	A	3	-	12,14,14	1.14	3 (25%)	12,19,19	0.67	0
2	SRO	A	1	-	12,14,14	1.10	2 (16%)	12,19,19	0.72	0
2	SRO	B	4	-	12,14,14	1.10	2 (16%)	12,19,19	0.79	0

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	SRO	A	3	-	-	2/3/3/3	0/2/2/2
2	SRO	A	1	-	-	1/3/3/3	0/2/2/2
2	SRO	B	4	-	-	1/3/3/3	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3	SRO	CZ2-CH2	2.24	1.41	1.36
2	A	1	SRO	CE3-CZ3	2.22	1.41	1.37
2	B	4	SRO	CE3-CZ3	2.18	1.41	1.37
2	A	3	SRO	CE3-CZ3	2.16	1.41	1.37
2	A	1	SRO	CZ2-CH2	2.14	1.41	1.36
2	A	3	SRO	CH2-CZ3	2.09	1.42	1.38
2	B	4	SRO	CZ2-CH2	2.06	1.40	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3	SRO	CA-CB-CG-CD2
2	A	3	SRO	NZ-CA-CB-CG
2	A	1	SRO	NZ-CA-CB-CG
2	B	4	SRO	NZ-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3	SRO	4	0



## 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	262/287 (91%)	0.45	22 (8%) 11 14	29, 45, 75, 99	0
1	B	257/287 (89%)	0.92	43 (16%) 1 2	29, 47, 100, 111	0
All	All	519/574 (90%)	0.69	65 (12%) 3 5	29, 46, 88, 111	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	265	LYS	8.2
1	B	363	PHE	7.8
1	A	261	LYS	7.0
1	B	264	PHE	6.6
1	B	459	THR	6.5
1	B	461	THR	5.8
1	A	358	LYS	5.3
1	B	275	LYS	5.2
1	A	263	LYS	5.1
1	B	456	ILE	5.1
1	B	271	GLN	4.9
1	B	262	ILE	4.4
1	B	360	PHE	4.1
1	B	458	LYS	4.0
1	A	262	ILE	3.8
1	B	358	LYS	3.7
1	A	260	ASP	3.6
1	B	243	ASP	3.6
1	A	287	PHE	3.5
1	B	266	HIS	3.5
1	A	427	GLU	3.4
1	B	357	ARG	3.3
1	B	283	GLN	3.3
1	B	245	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	259	GLU	3.3
1	A	256	MET	3.2
1	A	258	GLY	3.2
1	B	256	MET	3.1
1	B	270	LEU	3.1
1	B	261	LYS	3.0
1	B	268	THR	3.0
1	B	207	GLU	3.0
1	B	355	SER	2.9
1	B	279	ILE	2.9
1	A	363	PHE	2.7
1	A	465	LEU	2.7
1	B	359	PRO	2.6
1	B	391	ILE	2.6
1	B	282	PHE	2.6
1	B	321	GLY	2.6
1	B	442	LEU	2.6
1	A	455	VAL	2.5
1	B	427	GLU	2.5
1	B	361	GLY	2.5
1	B	455	VAL	2.5
1	A	356	LEU	2.4
1	B	328	THR	2.4
1	A	241	THR	2.4
1	B	460	GLU	2.4
1	B	325	ILE	2.3
1	B	352	PHE	2.3
1	A	207	GLU	2.3
1	B	255	LEU	2.3
1	B	439	MET	2.3
1	B	277	VAL	2.2
1	B	423	LEU	2.2
1	A	362	ASP	2.2
1	A	204	LEU	2.1
1	A	252	MET	2.1
1	A	282	PHE	2.1
1	B	244	LYS	2.1
1	A	456	ILE	2.1
1	B	252	MET	2.1
1	B	470	GLN	2.1
1	A	426	PRO	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SRO	A	3	13/13	0.47	0.52	79,84,85,85	0
2	SRO	A	1	13/13	0.76	0.33	83,85,86,86	0
2	SRO	B	4	13/13	0.78	0.24	91,93,94,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.