



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:10 AM GMT

PDB ID : 2POB
Title : PPARgamma Ligand binding domain complexed with a farglitazar analogue gw4709
Authors : Nolte, R.T.
Deposited on : 2007-04-26
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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

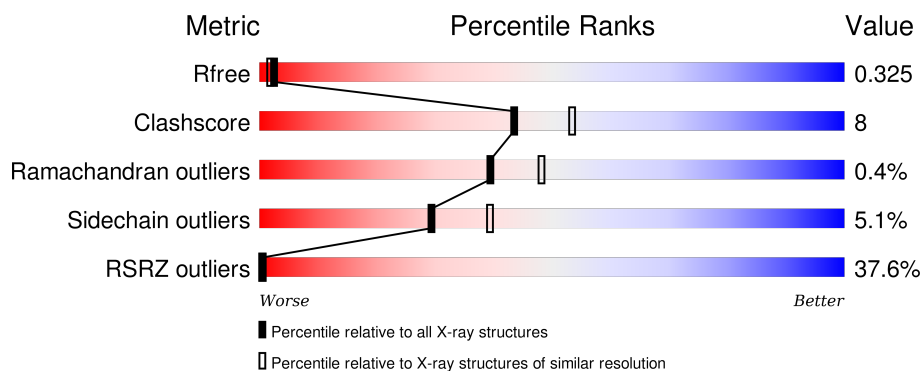
1 Overall quality at a glance

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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 ≥ 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>36%</div> <div>75%</div> <div>17%</div> <div>6%</div> </div>
1	B	272	<div> <div>34%</div> <div>73%</div> <div>18%</div> <div>9%</div> </div>

2 Entry composition [i](#)

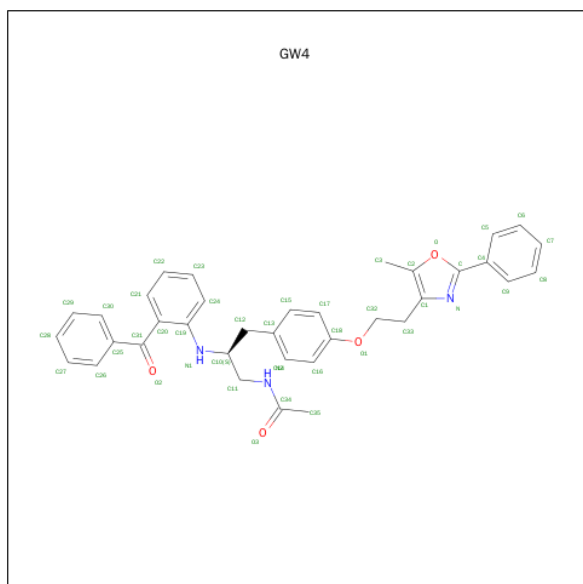
There are 4 unique types of molecules in this entry. The entry contains 4278 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	255	Total	C	N	O	S	0	2	0
			2037	1312	332	384	9			
1	B	247	Total	C	N	O	S	0	3	0
			1971	1269	323	370	9			

- Molecule 2 is N-[(2S)-2-[(2-BENZOYLPHENYL)AMINO]-3-{4-[2-(5-METHYL-2-PHENYL-1,3-OXAZOL-4-YL)ETHOXY]PHENYL}PROPYL]ACETAMIDE (three-letter code: GW4) (formula: C₃₆H₃₅N₃O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			43	36	3	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		

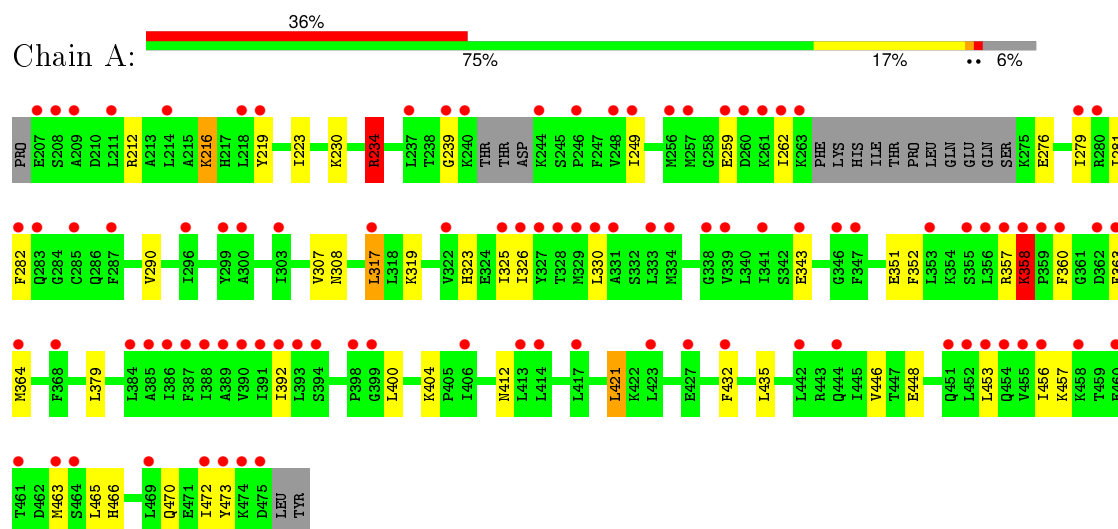
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	125	Total	O	0	0
			125	125		
4	B	96	Total	O	0	0
			96	96		

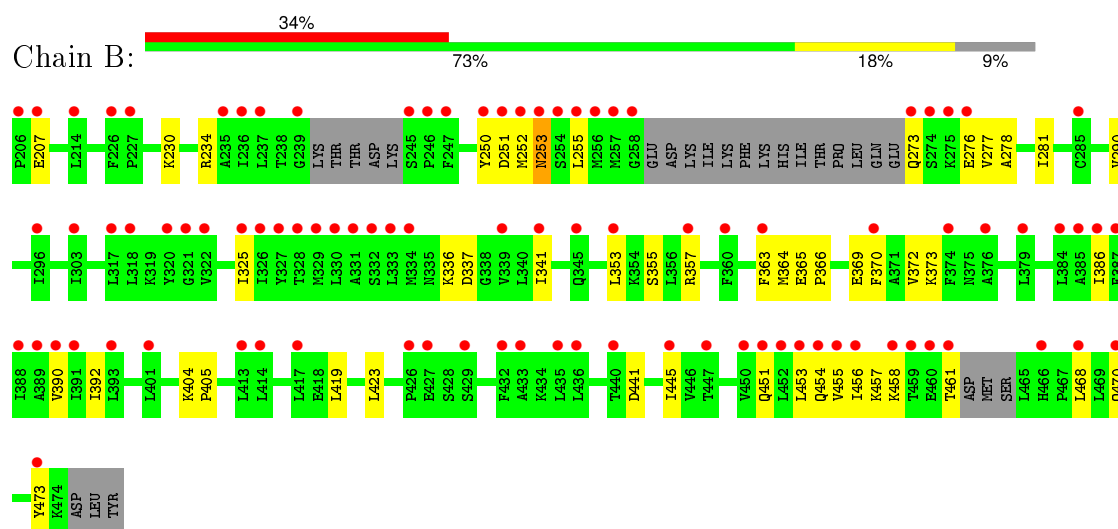
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.92Å 62.01Å 118.17Å 90.00° 101.94° 90.00°	Depositor
Resolution (Å)	24.50 – 2.30 24.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.0 (24.50-2.30) 91.0 (24.16-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.273 0.280 , 0.325	Depositor DCC
R_{free} test set	875 reflections (3.38%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 71.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26798 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4278	wwPDB-VP
Average B, all atoms (Å ²)	75.0	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, GW4

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	0.57	2/2069 (0.1%)	0.63	1/2790 (0.0%)
1	B	0.59	2/2003 (0.1%)	0.65	1/2705 (0.0%)
All	All	0.58	4/4072 (0.1%)	0.64	2/5495 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	337	ASP	CG-OD2	7.51	1.42	1.25
1	B	336	LYS	CE-NZ	5.52	1.62	1.49
1	A	308	ASN	CG-ND2	5.33	1.46	1.32
1	A	308	ASN	CG-OD1	5.05	1.35	1.24

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	337	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	234	ARG	NE-CZ-NH2	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	358	LYS	Peptide

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	2037	0	2059	37	0
1	B	1971	0	1972	30	0
2	A	43	0	35	7	0
3	B	6	0	8	1	0
4	A	125	0	0	1	0
4	B	96	0	0	0	0
All	All	4278	0	4074	66	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 8.

All (66) 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:255:LEU:HD11	1:B:281:ILE:HD11	1.32	1.07
1:B:255:LEU:CD1	1:B:281:ILE:HD11	1.89	1.01
1:B:453:LEU:O	1:B:456:ILE:HG22	1.74	0.87
1:B:419:LEU:O	1:B:423:LEU:HD13	1.82	0.79
1:A:472:ILE:CD1	1:B:468:LEU:HD11	2.20	0.72
1:B:276:GLU:OE1	1:B:278:ALA:HB3	1.90	0.72
1:A:323:HIS:ND1	2:A:478:GW4:H352	2.09	0.68
1:B:250:TYR:CD2	1:B:251:ASP:HB2	2.29	0.68
1:A:219:TYR:O	1:A:223:ILE:HD12	1.94	0.67
1:A:453:LEU:HD11	1:A:473:TYR:CZ	2.31	0.66
1:B:370:PHE:HB2	1:B:445:ILE:HD11	1.77	0.66
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.77	0.65
1:B:455:VAL:O	1:B:455:VAL:HG12	1.99	0.61
1:A:465:LEU:HB3	1:A:470:GLN:HE21	1.65	0.60
1:A:319:LYS:HA	1:A:472:ILE:HD12	1.85	0.59
2:A:478:GW4:C30	2:A:478:GW4:H21	2.31	0.58
1:A:219:TYR:CE1	1:A:223:ILE:HD11	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ILE:HD13	1:B:468:LEU:HD11	1.87	0.55
1:A:249:ILE:HD11	1:A:262:ILE:HD11	1.89	0.55
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.86	0.55
1:A:472:ILE:HD11	1:B:468:LEU:HD11	1.89	0.55
1:A:230:LYS:O	1:A:234:ARG:HG2	2.07	0.55
1:A:421:LEU:HD23	1:A:432:PHE:HA	1.90	0.54
1:B:451:GLN:O	1:B:455:VAL:HG23	2.07	0.53
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.38	0.52
1:A:323:HIS:NE2	1:A:472:ILE:HG22	2.24	0.51
1:B:250:TYR:CE2	1:B:251:ASP:HB2	2.46	0.51
1:A:330:LEU:HD21	1:A:364:MET:HE3	1.93	0.50
1:A:323:HIS:HB3	1:A:446:VAL:HG22	1.93	0.50
1:A:326:ILE:HD12	2:A:478:GW4:H353	1.93	0.50
1:A:276:GLU:OE1	1:A:279:ILE:HD13	2.12	0.49
2:A:478:GW4:C21	2:A:478:GW4:C30	2.90	0.49
1:B:454:GLN:C	1:B:456:ILE:H	2.16	0.48
1:A:453:LEU:HD11	1:A:473:TYR:CE2	2.48	0.48
1:A:456:ILE:HG22	1:A:457:LYS:N	2.29	0.48
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.95	0.48
1:B:251:ASP:OD2	1:B:252:MET:N	2.46	0.48
1:A:358:LYS:O	1:A:358:LYS:HG3	2.14	0.48
1:B:253:ASN:ND2	1:B:253:ASN:O	2.44	0.48
1:A:317:LEU:HD13	1:A:400:LEU:HD21	1.96	0.47
1:B:457:LYS:O	1:B:461:THR:HG23	2.15	0.47
1:A:276:GLU:HA	1:A:279:ILE:HD13	1.96	0.47
1:A:363:PHE:CE2	2:A:478:GW4:H26	2.50	0.47
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.50	0.47
1:B:255:LEU:HD11	1:B:281:ILE:CD1	2.24	0.46
1:B:252:MET:SD	1:B:277:VAL:HG21	2.56	0.46
1:A:453:LEU:CD1	1:A:473:TYR:CZ	2.99	0.45
1:A:282:PHE:HD2	2:A:478:GW4:C29	2.31	0.44
1:A:358:LYS:O	1:A:358:LYS:CG	2.66	0.44
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.53	0.43
1:A:363:PHE:CE2	2:A:478:GW4:C26	3.02	0.43
1:A:307:VAL:HG13	4:A:497:HOH:O	2.19	0.43
1:A:319:LYS:HA	1:A:472:ILE:CD1	2.47	0.43
1:A:281:ILE:HD11	1:A:352:PHE:HE2	1.84	0.42
1:B:456:ILE:CG2	1:B:457:LYS:N	2.83	0.42
1:B:404:LYS:N	1:B:405:PRO:HD2	2.35	0.42
1:A:212:ARG:O	1:A:216:LYS:HD3	2.20	0.42
1:B:386:ILE:O	1:B:390:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ILE:HB	3:B:478:GOL:H12	2.02	0.42
1:B:353:LEU:HD13	1:B:364:MET:HG3	2.01	0.42
1:A:290:VAL:HG21	1:A:466:HIS:CG	2.56	0.40
1:B:365:GLU:HB3	1:B:366:PRO:HD3	2.03	0.40
1:A:230:LYS:O	1:A:234:ARG:CG	2.69	0.40
1:A:360:PHE:CE1	1:A:456:ILE:HD11	2.56	0.40
1:B:230:LYS:O	1:B:234:ARG:HG2	2.21	0.40
1:B:369:GLU:O	1:B:372:VAL:HG12	2.22	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	251/272 (92%)	240 (96%)	10 (4%)	1 (0%)	39	48
1	B	242/272 (89%)	237 (98%)	4 (2%)	1 (0%)	39	48
All	All	493/544 (91%)	477 (97%)	14 (3%)	2 (0%)	39	48

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	B	458	LYS

5.3.2 Protein sidechains [i](#)

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	224/245 (91%)	211 (94%)	13 (6%)	25	33
1	B	215/245 (88%)	205 (95%)	10 (5%)	32	43
All	All	439/490 (90%)	416 (95%)	23 (5%)	29	38

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	234	ARG
1	A	259	GLU
1	A	317	LEU
1	A	343	GLU
1	A	351	GLU
1	A	357	ARG
1	A	358	LYS
1	A	404	LYS
1	A	412	ASN
1	A	421	LEU
1	A	448	GLU
1	A	463	MET
1	B	207[A]	GLU
1	B	207[B]	GLU
1	B	253	ASN
1	B	273	GLN
1	B	355	SER
1	B	357	ARG
1	B	363	PHE
1	B	373	LYS
1	B	441	ASP
1	B	470	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	ASN
1	A	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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GW4	A	478	-	43,47,47	0.83	1 (2%)	54,63,63	1.63	9 (16%)
3	GOL	B	478	-	5,5,5	0.34	0	5,5,5	0.32	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	GW4	A	478	-	-	0/28/31/31	0/4/5/5
3	GOL	B	478	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	478	GW4	C19-N1	2.33	1.42	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	478	GW4	C19-N1-C10	-6.14	115.63	125.03
2	A	478	GW4	C35-C34-N2	-2.77	111.97	116.19
2	A	478	GW4	C32-O1-C18	-2.55	111.64	117.91
2	A	478	GW4	C24-C19-C20	-2.53	115.82	119.41
2	A	478	GW4	C13-C12-C10	-2.32	109.31	114.32
2	A	478	GW4	C21-C20-C19	2.47	121.80	118.81
2	A	478	GW4	O3-C34-N2	2.72	126.64	121.79
2	A	478	GW4	C4-C-N	4.28	129.71	123.72
2	A	478	GW4	C3-C2-C1	4.35	134.85	127.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	478	GW4	7	0
3	B	478	GOL	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	255/272 (93%)	1.85	97 (38%) 0 0	61, 73, 88, 100	0
1	B	247/272 (90%)	1.91	92 (37%) 0 0	66, 74, 93, 107	0
All	All	502/544 (92%)	1.88	189 (37%) 0 0	61, 74, 90, 107	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	456	ILE	9.2
1	A	262	ILE	7.9
1	A	461	THR	7.1
1	B	256	MET	7.0
1	B	274	SER	6.8
1	B	273	GLN	6.0
1	B	275	LYS	6.0
1	B	239	GLY	5.8
1	B	459	THR	5.5
1	A	362	ASP	5.3
1	A	390	VAL	5.2
1	B	235	ALA	5.2
1	B	236	ILE	5.1
1	A	391	ILE	5.0
1	B	384	LEU	4.9
1	B	245	SER	4.8
1	A	393	LEU	4.7
1	B	455	VAL	4.7
1	A	388	ILE	4.7
1	A	357	ARG	4.6
1	B	255	LEU	4.6
1	A	458	LYS	4.5
1	A	239	GLY	4.5
1	A	325	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	387	PHE	4.5
1	A	261	LYS	4.4
1	A	473	TYR	4.4
1	B	390	VAL	4.4
1	B	466	HIS	4.4
1	B	253	ASN	4.4
1	B	363	PHE	4.3
1	B	257	MET	4.3
1	A	339	VAL	4.3
1	B	458	LYS	4.2
1	A	285	CYS	4.2
1	A	330	LEU	4.2
1	A	389	ALA	4.2
1	B	258	GLY	4.1
1	B	325	ILE	4.1
1	A	300	ALA	4.1
1	B	252	MET	4.0
1	B	452	LEU	4.0
1	B	276	GLU	4.0
1	A	392	ILE	3.9
1	B	386	ILE	3.9
1	A	413	LEU	3.9
1	A	299	TYR	3.9
1	B	451	GLN	3.9
1	B	391	ILE	3.9
1	A	387	PHE	3.8
1	A	451	GLN	3.8
1	A	260	ASP	3.8
1	B	389	ALA	3.7
1	A	384	LEU	3.7
1	B	427	GLU	3.7
1	A	341	ILE	3.7
1	B	388	ILE	3.6
1	A	218	LEU	3.6
1	A	237	LEU	3.6
1	B	247	PHE	3.6
1	A	211	LEU	3.6
1	A	326	ILE	3.5
1	A	453	LEU	3.5
1	B	436	LEU	3.5
1	A	385	ALA	3.5
1	A	328	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	333	LEU	3.4
1	B	328	THR	3.4
1	B	251	ASP	3.4
1	B	207[A]	GLU	3.4
1	B	296	ILE	3.4
1	B	426	PRO	3.4
1	A	386	ILE	3.3
1	A	303	ILE	3.2
1	B	339	VAL	3.2
1	A	454	GLN	3.2
1	B	329	MET	3.2
1	B	417	LEU	3.2
1	A	464	SER	3.2
1	A	452	LEU	3.2
1	B	318	LEU	3.2
1	A	355	SER	3.2
1	A	256	MET	3.2
1	A	417	LEU	3.1
1	B	330	LEU	3.1
1	A	296	ILE	3.1
1	A	331	ALA	3.1
1	B	385	ALA	3.1
1	A	356	LEU	3.1
1	A	287	PHE	3.1
1	A	263	LYS	3.0
1	B	322	VAL	3.0
1	B	414	LEU	3.0
1	B	461	THR	3.0
1	A	209	ALA	3.0
1	A	259	GLU	3.0
1	A	474	LYS	2.9
1	A	249	ILE	2.9
1	A	414	LEU	2.9
1	B	470	GLN	2.9
1	B	435	LEU	2.9
1	B	460	GLU	2.9
1	A	364	MET	2.9
1	A	322	VAL	2.8
1	B	353	LEU	2.8
1	B	250	TYR	2.8
1	B	327	TYR	2.8
1	A	472	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	244	LYS	2.8
1	A	358	LYS	2.8
1	B	360	PHE	2.7
1	B	374	PHE	2.7
1	A	427	GLU	2.7
1	A	240	LYS	2.7
1	A	334	MET	2.7
1	A	280	ARG	2.7
1	A	360	PHE	2.6
1	A	279	ILE	2.6
1	B	473	TYR	2.6
1	A	398	PRO	2.6
1	B	321	GLY	2.6
1	A	347	PHE	2.5
1	A	208	SER	2.5
1	B	303	ILE	2.5
1	B	429	SER	2.5
1	B	214	LEU	2.4
1	B	237	LEU	2.4
1	B	453	LEU	2.4
1	B	376	ALA	2.4
1	B	326	ILE	2.4
1	B	432	PHE	2.4
1	B	393	LEU	2.4
1	A	327	TYR	2.4
1	B	320	TYR	2.4
1	A	406	ILE	2.4
1	B	445	ILE	2.4
1	B	226	PHE	2.4
1	B	341	ILE	2.4
1	B	331	ALA	2.4
1	B	454	GLN	2.4
1	B	254	SER	2.4
1	B	447	THR	2.4
1	B	317	LEU	2.3
1	A	455	VAL	2.3
1	B	450	VAL	2.3
1	A	338	GLY	2.3
1	A	463	MET	2.3
1	A	246	PRO	2.3
1	B	433	ALA	2.3
1	A	283	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	2.3
1	B	379	LEU	2.3
1	A	346	GLY	2.3
1	A	475	ASP	2.3
1	A	343	GLU	2.3
1	A	248	VAL	2.3
1	A	432	PHE	2.2
1	A	359	PRO	2.2
1	B	246	PRO	2.2
1	A	394	SER	2.2
1	B	370	PHE	2.2
1	A	399	GLY	2.2
1	A	442	LEU	2.2
1	B	401	LEU	2.2
1	B	413	LEU	2.2
1	B	206	PRO	2.2
1	B	440	THR	2.2
1	A	456	ILE	2.1
1	B	345	GLN	2.1
1	A	460	GLU	2.1
1	A	368	PHE	2.1
1	A	317	LEU	2.1
1	A	353	LEU	2.1
1	B	468	LEU	2.1
1	A	207	GLU	2.1
1	A	257	MET	2.1
1	B	332	SER	2.1
1	A	219	TYR	2.1
1	A	329	MET	2.1
1	B	333	LEU	2.1
1	A	282	PHE	2.0
1	A	363	PHE	2.0
1	A	423	LEU	2.0
1	A	469	LEU	2.0
1	B	334	MET	2.0
1	A	444	GLN	2.0
1	B	227	PRO	2.0
1	B	285	CYS	2.0
1	B	357	ARG	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	B	478	6/6	0.77	0.21	-0.21	56,61,62,62	0
2	GW4	A	478	43/43	0.85	0.23	-0.52	61,71,80,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.