



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:05 AM GMT

PDB ID : 2G0G
Title : Structure-based drug design of a novel family of PPAR partial agonists: virtual screening, x-ray crystallography and in vitro/in vivo biological activities
Authors : Lu, I.L.; Peng, Y.H.; Huang, C.F.; Lin, Y.T.; Hsu, J.T.A.; Wu, S.Y.
Deposited on : 2006-02-13
Resolution : 2.54 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

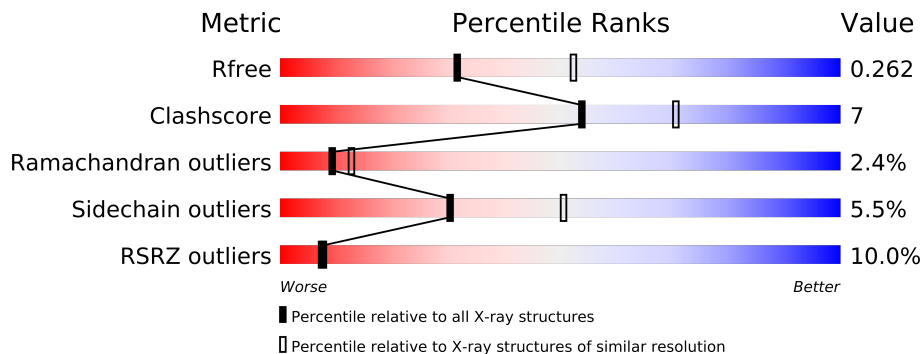
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.54 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}	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	271	
1	B	271	

2 Entry composition i

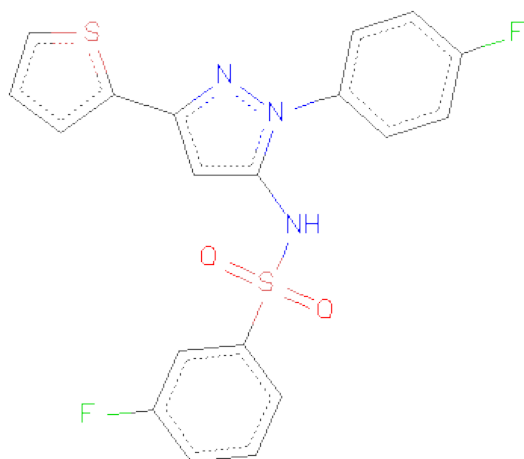
There are 3 unique types of molecules in this entry. The entry contains 4472 atoms, of which 0 are hydrogen and 0 are deuterium.

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	271	Total	C	N	O	S	0	0	0
			2177	1406	355	406	10			
1	B	271	Total	C	N	O	S	0	0	0
			2177	1406	355	406	10			

- Molecule 2 is 3-FLUORO-N-[1-(4-FLUOROPHENYL)-3-(2-THIENYL)-1H-PYRAZOL-5-YL]BENZENESULFONAMIDE (three-letter code: SP0) (formula: C₁₉H₁₃F₂N₃O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	19	2	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		

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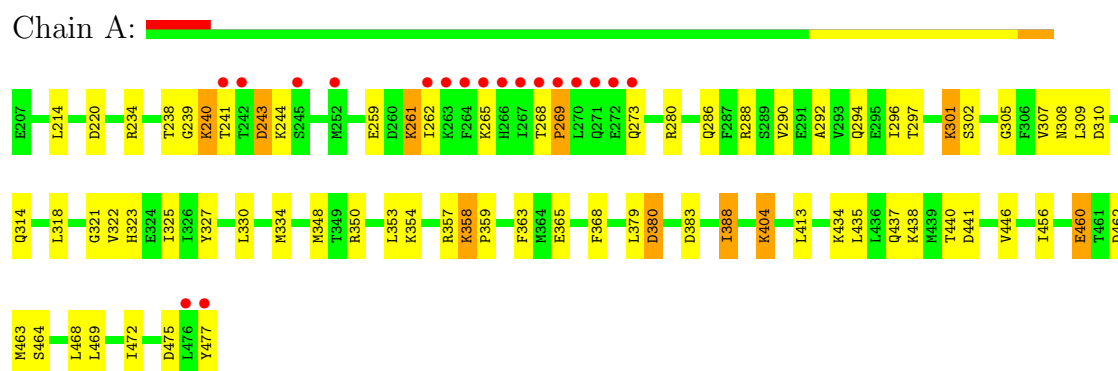
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	58	Total	O	0	0
			58	58		

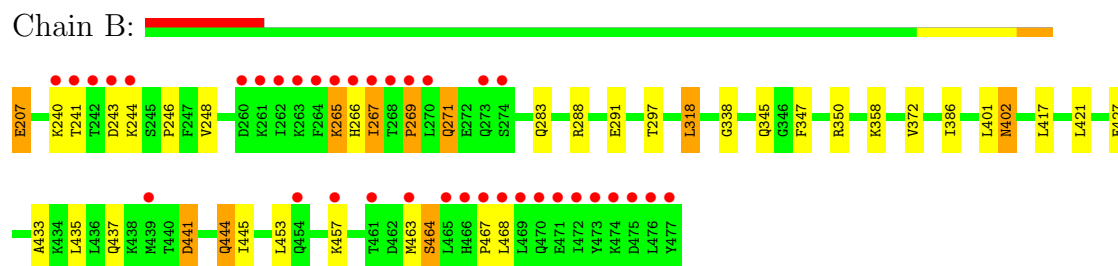
3 Residue-property plots

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-activatedreceptor gamma



- Molecule 1: Peroxisome proliferator-activatedreceptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.42Å 88.81Å 58.26Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	20.00 – 2.54 29.94 – 2.54	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.54) 99.1 (29.94-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.216 , 0.264 0.219 , 0.262	Depositor DCC
R_{free} test set	975 reflections (5.45%)	DCC
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.0	EDS
Estimated twinning fraction	0.000 for -l,k,h 0.033 for h,-k,-l 0.027 for -l,-k,-h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 18864 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4472	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SP0

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	0.39	0/2215	0.98	4/2985 (0.1%)
1	B	0.41	0/2215	0.97	3/2985 (0.1%)
All	All	0.40	0/4430	0.98	7/5970 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	GLU	OE1-CD-OE2	6.62	131.24	123.30
1	A	404	LYS	CD-CE-NZ	6.05	125.63	111.70
1	B	350	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	380	ASP	CB-CG-OD1	5.39	123.16	118.30
1	A	388	ILE	CG1-CB-CG2	-5.22	99.91	111.40
1	B	207	GLU	CG-CD-OE2	-5.18	107.94	118.30
1	A	301	LYS	CD-CE-NZ	5.16	123.57	111.70

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2177	0	2241	40	0
1	B	2177	0	2241	22	0
2	A	28	0	13	1	0
3	A	32	0	0	3	0
3	B	58	0	0	4	0
All	All	4472	0	4495	61	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (61) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:354:LYS:HE2	1:A:365:GLU:HG2	1.57	0.86
1:A:325:ILE:HD12	1:A:388:ILE:HG13	1.61	0.82
1:A:327:TYR:HE2	1:A:446:VAL:HG22	1.54	0.72
1:B:421:LEU:HD11	1:B:435:LEU:HD23	1.75	0.69
1:A:292:ALA:O	1:A:296:ILE:HG12	1.93	0.69
1:B:240:LYS:HG3	1:B:241:THR:HG22	1.78	0.65
1:B:401:LEU:C	1:B:402:ASN:HD22	2.02	0.62
1:A:296:ILE:HD12	1:A:325:ILE:HG21	1.82	0.62
1:A:350:ARG:HG3	1:A:368:PHE:CD2	2.34	0.62
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.82	0.61
1:A:434:LYS:HA	1:A:437:GLN:HE21	1.68	0.59
1:B:402:ASN:N	1:B:402:ASN:HD22	2.02	0.57
1:B:288:ARG:HH11	1:B:291:GLU:HB3	1.70	0.57
1:B:444:GLN:HB3	3:B:72:HOH:O	2.03	0.57
1:B:433:ALA:O	1:B:437:GLN:HG3	2.06	0.55
1:A:214:LEU:HD21	1:A:413:LEU:HD23	1.89	0.54
1:B:402:ASN:N	1:B:402:ASN:ND2	2.54	0.53
1:A:261:LYS:HE3	1:A:261:LYS:HA	1.90	0.53
1:A:297:THR:HG23	1:A:318:LEU:HD21	1.92	0.52
1:B:441:ASP:O	1:B:445:ILE:HD12	2.09	0.52
1:A:290:VAL:HG13	1:A:468:LEU:HD23	1.93	0.51
1:B:265:LYS:HG3	1:B:266:HIS:H	1.76	0.51
1:A:327:TYR:CE2	1:A:446:VAL:HG22	2.42	0.51
1:A:348:MET:SD	1:A:353:LEU:HD21	2.51	0.49
1:A:321:GLY:O	1:A:325:ILE:HG12	2.12	0.49
1:B:297:THR:HG23	1:B:318:LEU:HD21	1.95	0.49
1:A:307:VAL:HG22	3:A:86:HOH:O	2.13	0.48
1:A:296:ILE:HD12	1:A:325:ILE:CG2	2.42	0.48
1:A:330:LEU:O	1:A:334:MET:HG3	2.13	0.48
1:B:386:ILE:HB	1:B:417:LEU:HD13	1.96	0.48
1:A:309:LEU:O	1:A:310:ASP:C	2.53	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:271:GLN:HG2	1:B:283:GLN:HE21	1.79	0.47
1:A:323:HIS:HE1	1:A:472:ILE:HG22	1.79	0.46
1:B:269:PRO:HA	3:B:88:HOH:O	2.16	0.46
2:A:101:SP0:H17	2:A:101:SP0:C16	2.29	0.46
1:B:372:VAL:HG12	3:B:28:HOH:O	2.15	0.46
1:A:301:LYS:CD	1:B:468:LEU:HB2	2.46	0.46
1:A:456:ILE:O	1:A:460:GLU:HB2	2.16	0.45
1:A:325:ILE:HG23	1:A:388:ILE:HG13	1.98	0.45
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.97	0.45
1:A:310:ASP:O	1:A:314:GLN:HG3	2.16	0.45
1:A:438:LYS:HE2	3:A:64:HOH:O	2.17	0.45
1:A:259:GLU:O	1:A:262:ILE:HG13	2.18	0.44
1:A:239:GLY:C	1:A:241:THR:H	2.20	0.44
1:B:463:MET:O	1:B:464:SER:HB2	2.18	0.44
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.53	0.43
1:B:271:GLN:HG2	1:B:283:GLN:NE2	2.33	0.43
1:A:325:ILE:HG23	1:A:388:ILE:CG1	2.49	0.43
1:A:290:VAL:O	1:A:294:GLN:HG3	2.19	0.42
1:B:244:LYS:HG2	3:B:90:HOH:O	2.18	0.42
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.85	0.42
1:A:404:LYS:NZ	3:A:50:HOH:O	2.52	0.42
1:A:259:GLU:C	1:A:261:LYS:H	2.23	0.41
1:A:301:LYS:NZ	1:B:467:PRO:HD2	2.36	0.41
1:A:290:VAL:HG22	1:A:469:LEU:HG	2.02	0.41
1:A:273:GLN:HA	1:A:280:ARG:CD	2.50	0.41
1:A:268:THR:HA	1:A:269:PRO:HD3	1.97	0.41
1:A:380:ASP:OD1	1:A:383:ASP:N	2.48	0.40
1:A:358:LYS:HB3	1:A:359:PRO:HD3	2.02	0.40
1:A:238:THR:CG2	1:A:240:LYS:HG3	2.52	0.40
1:B:246:PRO:HA	1:B:345:GLN:O	2.21	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	269/271 (99%)	247 (92%)	15 (6%)	7 (3%)	8	11
1	B	269/271 (99%)	242 (90%)	21 (8%)	6 (2%)	10	15
All	All	538/542 (99%)	489 (91%)	36 (7%)	13 (2%)	9	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	358	LYS
1	A	475	ASP
1	B	464	SER
1	A	240	LYS
1	B	265	LYS
1	B	267	ILE
1	A	243	ASP
1	A	269	PRO
1	A	464	SER
1	B	269	PRO
1	B	271	GLN
1	B	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	244/244 (100%)	228 (93%)	16 (7%)	24	40
1	B	244/244 (100%)	233 (96%)	11 (4%)	38	61
All	All	488/488 (100%)	461 (94%)	27 (6%)	30	50

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	ASP
1	A	234	ARG
1	A	243	ASP
1	A	261	LYS

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Mol	Chain	Res	Type
1	A	265	LYS
1	A	286	GLN
1	A	288	ARG
1	A	302	SER
1	A	322	VAL
1	A	363	PHE
1	A	440	THR
1	A	441	ASP
1	A	460	GLU
1	A	462	ASP
1	A	463	MET
1	A	477	TYR
1	B	207	GLU
1	B	243	ASP
1	B	248	VAL
1	B	267	ILE
1	B	318	LEU
1	B	402	ASN
1	B	427	GLU
1	B	441	ASP
1	B	444	GLN
1	B	453	LEU
1	B	457	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	294	GLN
1	A	308	ASN
1	A	312	ASN
1	A	437	GLN
1	A	444	GLN
1	A	451	GLN
1	B	271	GLN
1	B	273	GLN
1	B	283	GLN
1	B	402	ASN
1	B	437	GLN
1	B	454	GLN
1	B	470	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	SP0	A	101	-	31,31,31	3.10	9 (29%)	45,45,45	3.53	14 (31%)

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	SP0	A	101	-	-	0/18/19/19	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	SP0	N7-N8	-8.76	1.23	1.39
2	A	101	SP0	C6-C4	-7.76	1.39	1.50
2	A	101	SP0	O19-S18	6.68	1.50	1.43
2	A	101	SP0	O20-S18	6.60	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	101	SP0	C11-N8	-4.63	1.34	1.43
2	A	101	SP0	C9-N8	-3.62	1.33	1.36
2	A	101	SP0	C10-C6	-3.61	1.33	1.40
2	A	101	SP0	C4-S3	-2.18	1.70	1.72
2	A	101	SP0	C9-N17	-2.11	1.33	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	101	SP0	C10-C9-N8	14.18	108.84	106.68
2	A	101	SP0	C2-S3-C4	9.53	96.10	91.91
2	A	101	SP0	C11-N8-N7	8.13	125.13	118.85
2	A	101	SP0	C1-C2-S3	-7.36	105.26	113.18
2	A	101	SP0	C5-C4-S3	-5.16	104.84	111.02
2	A	101	SP0	O20-S18-O19	-4.14	113.98	119.55
2	A	101	SP0	N17-C9-N8	3.79	124.86	120.99
2	A	101	SP0	C4-C6-N7	3.74	126.02	120.72
2	A	101	SP0	C6-N7-N8	3.02	110.26	105.19
2	A	101	SP0	C21-S18-N17	2.66	109.96	106.81
2	A	101	SP0	O19-S18-N17	2.45	112.99	106.72
2	A	101	SP0	F40-C23-C24	2.26	122.63	118.52
2	A	101	SP0	C24-C23-C22	-2.13	120.39	123.32
2	A	101	SP0	C1-C5-C4	2.07	117.31	110.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	271/271 (100%)	0.29	18 (6%) 18 18	27, 48, 107, 138	0
1	B	271/271 (100%)	0.58	36 (13%) 4 3	22, 40, 132, 158	0
All	All	542/542 (100%)	0.44	54 (9%) 8 7	22, 44, 123, 158	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	THR	13.8
1	B	476	LEU	12.4
1	B	477	TYR	11.9
1	A	269	PRO	9.9
1	B	468	LEU	9.5
1	B	470	GLN	9.3
1	B	473	TYR	9.2
1	B	472	ILE	8.5
1	A	267	ILE	8.0
1	B	264	PHE	7.9
1	B	471	GLU	7.8
1	B	465	LEU	6.9
1	B	267	ILE	6.8
1	A	266	HIS	6.5
1	A	477	TYR	6.4
1	A	273	GLN	6.0
1	B	241	THR	5.6
1	B	474	LYS	5.3
1	B	274	SER	5.2
1	B	273	GLN	4.7
1	B	467	PRO	4.5
1	B	266	HIS	4.3
1	A	264	PHE	4.1
1	A	268	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	4.1
1	B	475	ASP	4.1
1	A	265	LYS	4.1
1	B	240	LYS	4.0
1	A	476	LEU	3.9
1	B	270	LEU	3.9
1	A	271	GLN	3.8
1	A	242	THR	3.8
1	B	265	LYS	3.6
1	B	263	LYS	3.5
1	B	243	ASP	3.5
1	B	260	ASP	3.3
1	B	244	LYS	3.2
1	B	242	THR	3.2
1	B	463	MET	3.1
1	A	272	GLU	3.0
1	B	469	LEU	3.0
1	A	262	ILE	2.9
1	B	262	ILE	2.7
1	A	245	SER	2.7
1	B	269	PRO	2.7
1	A	241	THR	2.6
1	B	261	LYS	2.6
1	B	461	THR	2.3
1	A	263	LYS	2.3
1	B	457	LYS	2.2
1	B	466	HIS	2.1
1	A	252	MET	2.1
1	B	454	GLN	2.1
1	B	439	MET	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. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SP0	A	101	28/28	0.17	0.08	78,82,85,89	0

6.5 Other polymers

There are no such residues in this entry.