



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 11:52 AM UTC

PDB ID : 6DHA / pdb_00006dha
Title : Crystal Structure of Human PPARgamma Ligand Binding Domain in Complex with Hydroxy Pioglitazone (M-IV)
Authors : Shang, J.; Mosure, S.A.; Kojetin, D.J.
Deposited on : 2018-05-18
Resolution : 1.88 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

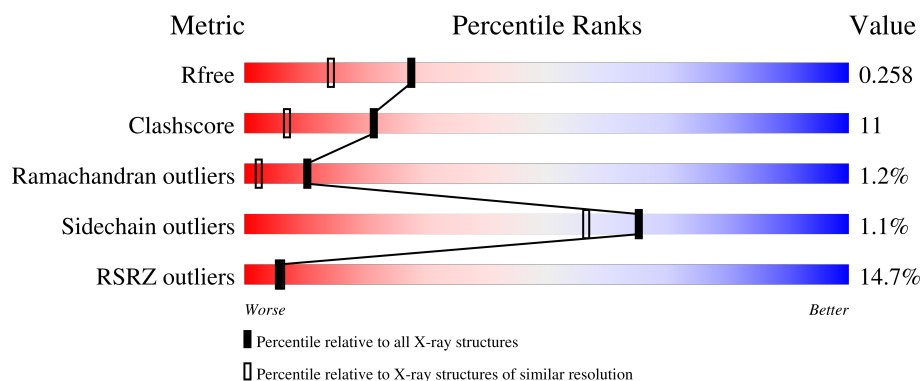
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	271	11% 79% 14% 6%
1	B	271	17% 76% 20% • •

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
3	KNA	A	502	-	-	X	-

2 Entry composition [i](#)

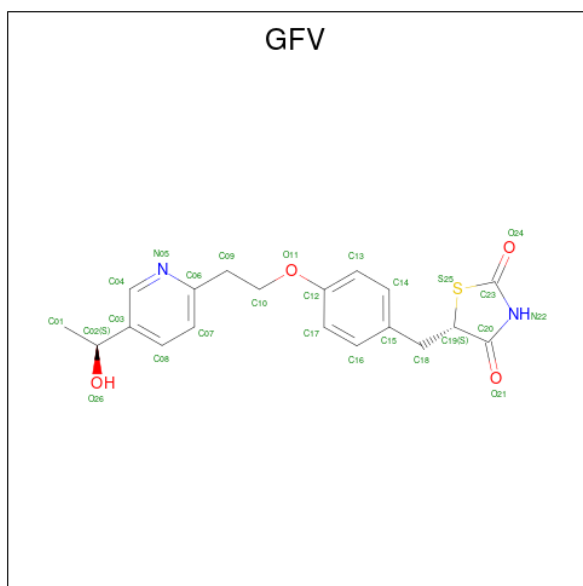
There are 4 unique types of molecules in this entry. The entry contains 4463 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

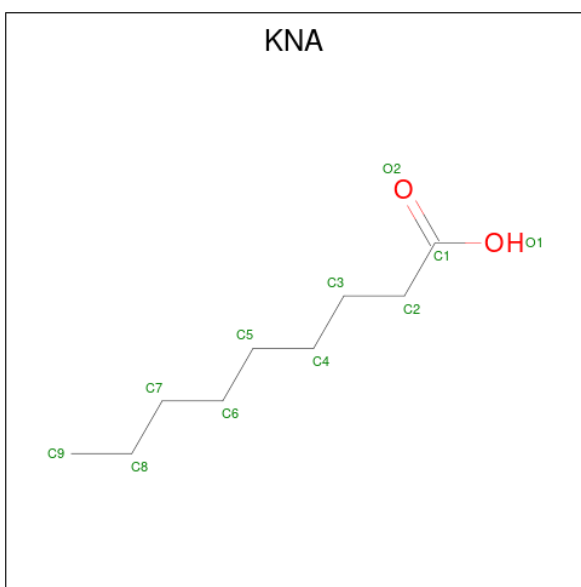
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2037	1313	331	383	10			
1	B	263	Total	C	N	O	S	0	0	0
			2108	1362	344	392	10			

- Molecule 2 is Hydroxy Pioglitazone (M-IV) (CCD ID: GFV) (formula: $C_{19}H_{20}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	19	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			26	19	2	4	1		

- Molecule 3 is nonanoic acid (CCD ID: KNA) (formula: $C_9H_{18}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	A	1	Total	C	O	0	0
			11	9	2		

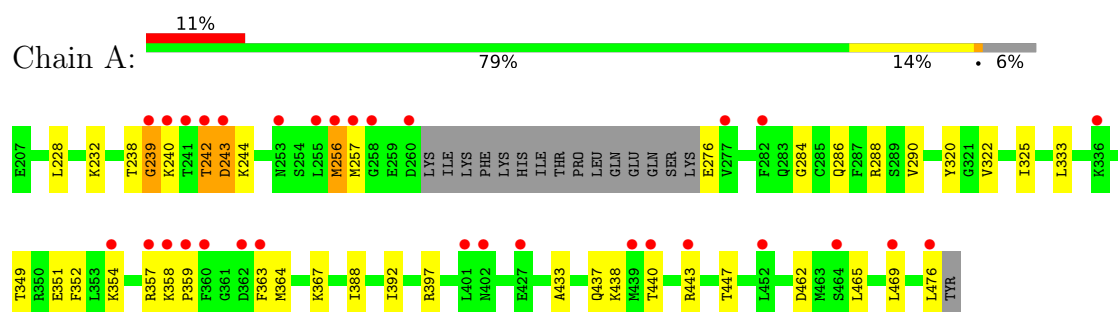
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	127	Total	O	0	0
			127	127		
4	B	117	Total	O	0	0
			117	117		

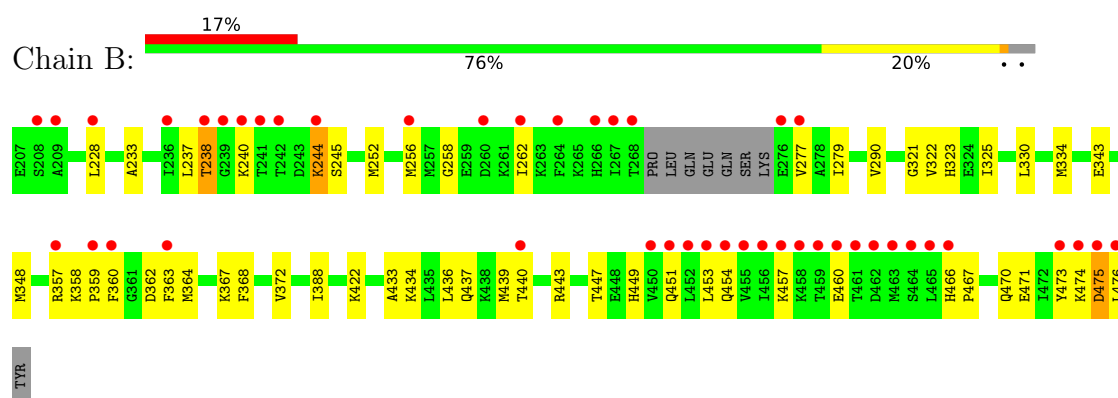
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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, α , β , γ	93.08Å 61.85Å 119.67Å 90.00° 102.73° 90.00°	Depositor
Resolution (Å)	51.12 – 1.88 51.12 – 1.88	Depositor EDS
% Data completeness (in resolution range)	97.3 (51.12-1.88) 97.3 (51.12-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.220 , 0.255 0.227 , 0.258	Depositor DCC
R_{free} test set	1981 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4463	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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, 0.333 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: GFV, KNA

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	0.35	0/2070	0.59	2/2790 (0.1%)
1	B	0.33	0/2143	0.55	0/2886
All	All	0.34	0/4213	0.57	2/5676 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASP	N-CA-C	-6.11	103.96	112.45
1	A	242	THR	CA-CB-OG1	-6.01	100.59	109.60

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	2037	0	2089	35	0
1	B	2108	0	2173	55	0
2	A	26	0	0	1	0
2	B	26	0	0	1	0
3	A	22	0	34	10	0
4	A	127	0	0	8	0
4	B	117	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4463	0	4296	93	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 11.

All (93) 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:357:ARG:NH1	1:B:359:PRO:HG2	1.68	1.08
1:B:357:ARG:HH12	1:B:359:PRO:HG2	1.08	1.07
1:B:357:ARG:NH2	1:B:360:PHE:HE2	1.72	0.86
1:A:239:GLY:O	1:A:242:THR:HG23	1.82	0.80
1:B:258:GLY:O	1:B:262:ILE:HG22	1.82	0.79
1:A:284:GLY:HA3	2:A:501:GFV:C01	2.16	0.76
1:A:357:ARG:HD2	1:A:359:PRO:HD2	1.69	0.75
1:B:357:ARG:NH1	1:B:359:PRO:CG	2.49	0.75
1:B:252:MET:HE1	1:B:277:VAL:HG21	1.68	0.74
1:B:325:ILE:HG23	1:B:388:ILE:HD12	1.72	0.72
1:B:238:THR:HB	4:B:645:HOH:O	1.89	0.71
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.74	0.70
1:A:288:ARG:CZ	3:A:502:KNA:H4A	2.22	0.70
1:A:288:ARG:NH1	3:A:502:KNA:H4A	2.07	0.69
1:A:440:THR:HG21	1:B:443:ARG:HD2	1.74	0.69
1:B:357:ARG:HG2	1:B:359:PRO:HD2	1.77	0.67
1:B:363:PHE:HE1	1:B:449:HIS:HE1	1.41	0.65
1:A:232:LYS:NZ	4:A:606:HOH:O	2.27	0.64
1:B:475:ASP:CG	1:B:476:LEU:HD23	2.22	0.64
1:A:357:ARG:CD	1:A:359:PRO:HD2	2.33	0.58
1:B:434:LYS:HG2	4:B:607:HOH:O	2.03	0.58
1:A:276:GLU:OE2	1:A:357:ARG:NH2	2.38	0.57
1:A:228:LEU:HD23	3:A:502:KNA:H2A	1.87	0.56
3:A:502:KNA:H7A	4:A:624:HOH:O	2.06	0.55
1:A:443:ARG:NH1	4:A:616:HOH:O	2.40	0.55
1:B:457:LYS:HD2	1:B:457:LYS:N	2.22	0.55
3:A:502:KNA:H2A	4:A:622:HOH:O	2.07	0.54
1:A:320:TYR:CE2	1:A:476:LEU:HD12	2.42	0.53
1:A:238:THR:O	1:A:240:LYS:N	2.41	0.53
1:B:466:HIS:N	1:B:467:PRO:HD3	2.23	0.53
1:A:349:THR:HG22	1:A:351:GLU:H	1.74	0.53
1:A:256:MET:C	1:A:256:MET:SD	2.93	0.52
1:B:322:VAL:HG21	1:B:476:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:GLN:NE2	4:B:607:HOH:O	2.42	0.52
1:B:228:LEU:HD21	1:B:233:ALA:HB2	1.93	0.51
1:B:466:HIS:HB3	1:B:470:GLN:CG	2.41	0.51
1:B:343:GLU:O	1:B:343:GLU:HG3	2.11	0.50
1:A:397:ARG:HH11	1:A:443:ARG:NH2	2.08	0.50
1:A:349:THR:HG22	1:A:351:GLU:N	2.27	0.49
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.95	0.49
1:B:368:PHE:O	1:B:372:VAL:HG22	2.12	0.48
1:B:322:VAL:CG2	1:B:476:LEU:HD12	2.43	0.48
1:B:358:LYS:NZ	1:B:362:ASP:OD1	2.46	0.48
1:A:367:LYS:NZ	4:A:618:HOH:O	2.45	0.48
1:B:357:ARG:NH2	1:B:360:PHE:CE2	2.65	0.48
1:B:363:PHE:CE1	1:B:449:HIS:HE1	2.28	0.47
1:B:357:ARG:NH1	1:B:359:PRO:CD	2.78	0.47
1:A:333:LEU:HD11	3:A:502:KNA:H8	1.97	0.47
1:A:433:ALA:O	1:A:437:GLN:HG3	2.14	0.47
1:B:451:GLN:O	1:B:454:GLN:HB3	2.13	0.47
1:B:323:HIS:HB2	4:B:615:HOH:O	2.14	0.47
1:B:228:LEU:CD2	1:B:233:ALA:HB2	2.44	0.46
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.97	0.46
1:B:334:MET:HE1	1:B:367:LYS:HB2	1.97	0.46
1:B:357:ARG:HH11	1:B:359:PRO:HD2	1.81	0.46
1:B:422:LYS:HA	1:B:422:LYS:HD3	1.71	0.46
1:B:358:LYS:NZ	1:B:362:ASP:OD2	2.49	0.46
1:B:321:GLY:O	1:B:325:ILE:HG12	2.16	0.46
1:B:357:ARG:NH2	1:B:460:GLU:OE1	2.49	0.46
1:A:238:THR:C	1:A:240:LYS:H	2.25	0.45
1:B:348:MET:HE1	2:B:501:GFV:C16	2.46	0.45
1:B:252:MET:O	1:B:256:MET:HG3	2.17	0.45
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.48	0.44
1:B:474:LYS:HD2	1:B:474:LYS:H	1.82	0.44
1:B:471:GLU:O	1:B:474:LYS:NZ	2.45	0.44
1:A:290:VAL:HG22	1:A:469:LEU:HD13	2.00	0.44
1:A:256:MET:SD	1:A:257:MET:N	2.91	0.44
1:A:443:ARG:O	1:A:447:THR:HG23	2.18	0.43
1:B:434:LYS:HA	1:B:437:GLN:HE21	1.83	0.43
1:B:357:ARG:HH11	1:B:359:PRO:CD	2.31	0.43
3:A:502:KNA:C1	4:A:622:HOH:O	2.65	0.43
1:B:357:ARG:CG	1:B:359:PRO:HD2	2.46	0.43
1:A:363:PHE:CZ	1:A:364:MET:HG2	2.54	0.43
1:A:440:THR:OG1	1:B:440:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:NH1	1:B:359:PRO:HD2	2.33	0.42
1:B:433:ALA:O	1:B:437:GLN:HG2	2.18	0.42
1:A:286:GLN:OE1	1:A:465:LEU:HD12	2.18	0.42
1:A:438:LYS:HD3	1:A:438:LYS:HA	1.87	0.42
3:A:503:KNA:H5	3:A:503:KNA:H8A	1.74	0.42
1:B:290:VAL:HG21	1:B:473:TYR:CE1	2.56	0.41
1:B:436:LEU:O	1:B:439:MET:HB2	2.19	0.41
1:A:228:LEU:CD2	3:A:502:KNA:H2A	2.50	0.41
1:A:462:ASP:OD2	4:A:601:HOH:O	2.22	0.41
1:B:244:LYS:HG3	4:B:619:HOH:O	2.20	0.41
1:A:349:THR:HG22	1:A:352:PHE:H	1.84	0.41
1:B:245:SER:HA	4:B:619:HOH:O	2.19	0.41
1:B:453:LEU:HA	1:B:453:LEU:HD12	1.85	0.41
3:A:502:KNA:H8	3:A:502:KNA:H5	1.59	0.41
1:B:252:MET:HE3	1:B:252:MET:HB3	1.89	0.41
1:B:447:THR:HG23	4:B:658:HOH:O	2.21	0.41
1:A:357:ARG:NH1	4:A:621:HOH:O	2.52	0.40
1:B:330:LEU:HD21	1:B:364:MET:HE1	2.02	0.40
1:B:279:ILE:H	1:B:279:ILE:HG13	1.67	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	251/271 (93%)	245 (98%)	5 (2%)	1 (0%)	30	18
1	B	259/271 (96%)	246 (95%)	8 (3%)	5 (2%)	6	0
All	All	510/542 (94%)	491 (96%)	13 (2%)	6 (1%)	10	2

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	B	237	LEU
1	B	244	LYS
1	B	475	ASP
1	B	240	LYS
1	B	238	THR

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	228/244 (93%)	223 (98%)	5 (2%)	45	30
1	B	236/244 (97%)	236 (100%)	0	100	100
All	All	464/488 (95%)	459 (99%)	5 (1%)	65	56

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243	ASP
1	A	244	LYS
1	A	256	MET
1	A	322	VAL
1	A	354	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	KNA	A	502	-	10,10,10	0.49	0	10,10,10	1.54	3 (30%)
2	GFV	B	501	-	28,28,28	5.59	13 (46%)	36,38,38	4.21	10 (27%)
2	GFV	A	501	-	28,28,28	5.57	13 (46%)	36,38,38	4.42	10 (27%)
3	KNA	A	503	-	10,10,10	0.77	0	10,10,10	1.14	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
3	KNA	A	502	-	-	5/8/8/8	-
2	GFV	B	501	-	-	4/14/26/26	0/3/3/3
2	GFV	A	501	-	-	0/14/26/26	0/3/3/3
3	KNA	A	503	-	-	7/8/8/8	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	GFV	C20-N22	20.42	1.64	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	GFV	C20-N22	20.39	1.64	1.37
2	A	501	GFV	C23-N22	11.72	1.51	1.36
2	B	501	GFV	C23-N22	11.59	1.51	1.36
2	B	501	GFV	C19-S25	-10.76	1.62	1.82
2	A	501	GFV	C19-S25	-10.56	1.62	1.82
2	A	501	GFV	C23-S25	-7.58	1.70	1.76
2	B	501	GFV	C23-S25	-7.45	1.70	1.76
2	B	501	GFV	O24-C23	-5.84	1.13	1.22
2	B	501	GFV	C19-C20	5.83	1.57	1.52
2	A	501	GFV	O24-C23	-5.78	1.13	1.22
2	A	501	GFV	C19-C20	5.48	1.57	1.52
2	B	501	GFV	C04-C03	4.99	1.46	1.39
2	A	501	GFV	C04-C03	4.87	1.45	1.39
2	B	501	GFV	C09-C10	4.24	1.64	1.51
2	A	501	GFV	C09-C10	4.12	1.64	1.51
2	B	501	GFV	O11-C12	3.19	1.44	1.37
2	A	501	GFV	O11-C12	3.17	1.44	1.37
2	A	501	GFV	C08-C07	2.69	1.43	1.38
2	B	501	GFV	C08-C07	2.62	1.43	1.38
2	B	501	GFV	C18-C15	2.56	1.57	1.51
2	A	501	GFV	C18-C15	2.38	1.56	1.51
2	B	501	GFV	O21-C20	-2.26	1.19	1.23
2	A	501	GFV	O21-C20	-2.26	1.19	1.23
2	A	501	GFV	O11-C10	-2.19	1.36	1.43
2	B	501	GFV	O11-C10	-2.17	1.36	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	GFV	C19-S25-C23	20.36	105.59	92.77
2	B	501	GFV	C19-S25-C23	17.09	103.53	92.77
2	B	501	GFV	C20-N22-C23	-15.43	107.90	118.20
2	A	501	GFV	C20-N22-C23	-13.76	109.02	118.20
2	B	501	GFV	S25-C23-N22	-5.48	106.59	110.44
2	A	501	GFV	S25-C23-N22	-4.22	107.48	110.44
2	B	501	GFV	C19-C20-N22	-3.96	108.64	111.99
2	A	501	GFV	C03-C04-N05	-3.50	120.21	124.47
2	A	501	GFV	C19-C20-N22	-3.48	109.05	111.99
2	B	501	GFV	C03-C04-N05	-3.19	120.59	124.47
2	A	501	GFV	C15-C18-C19	-3.09	108.91	113.35
3	A	502	KNA	O1-C1-C2	2.91	123.20	114.00
2	B	501	GFV	C07-C08-C03	-2.91	118.28	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	GFV	C04-N05-C06	2.86	121.64	118.00
2	B	501	GFV	O21-C20-C19	2.70	125.88	123.12
2	A	501	GFV	C08-C03-C04	2.70	119.67	116.89
2	A	501	GFV	C07-C08-C03	-2.69	118.50	121.18
2	B	501	GFV	C04-N05-C06	2.58	121.28	118.00
2	B	501	GFV	C08-C03-C04	2.57	119.54	116.89
2	B	501	GFV	O24-C23-S25	2.57	126.94	124.61
2	A	501	GFV	O21-C20-C19	2.31	125.48	123.12
3	A	502	KNA	O2-C1-C2	-2.10	116.44	123.09
3	A	502	KNA	C3-C2-C1	-2.02	109.25	114.51

There are no chirality outliers.

All (16) torsion outliers are listed below:

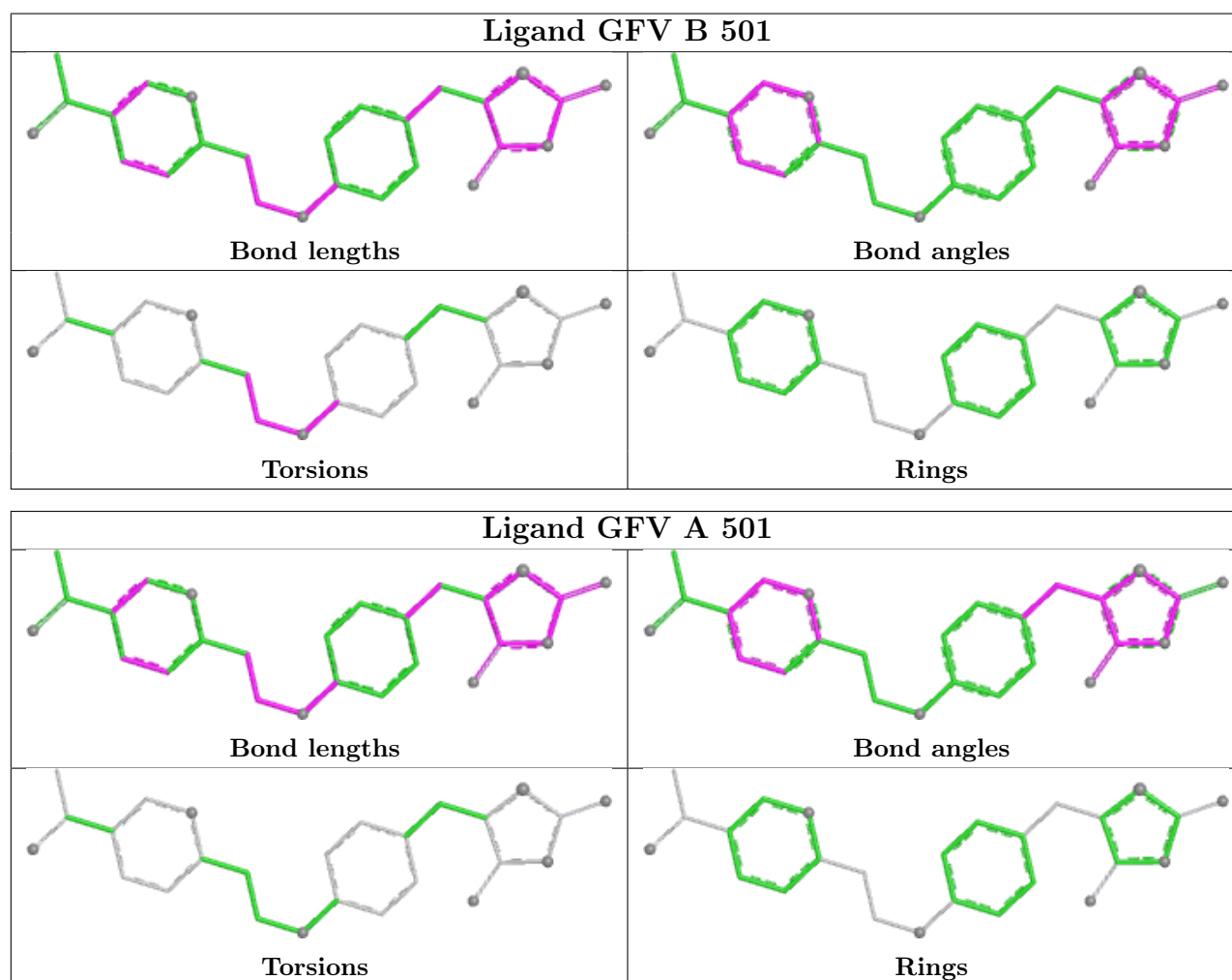
Mol	Chain	Res	Type	Atoms
3	A	503	KNA	C1-C2-C3-C4
3	A	502	KNA	C1-C2-C3-C4
3	A	503	KNA	C2-C3-C4-C5
3	A	502	KNA	C4-C5-C6-C7
2	B	501	GFV	C17-C12-O11-C10
3	A	502	KNA	C5-C6-C7-C8
2	B	501	GFV	C13-C12-O11-C10
3	A	503	KNA	C4-C5-C6-C7
2	B	501	GFV	C09-C10-O11-C12
3	A	502	KNA	C6-C7-C8-C9
3	A	503	KNA	C5-C6-C7-C8
2	B	501	GFV	C06-C09-C10-O11
3	A	502	KNA	C3-C4-C5-C6
3	A	503	KNA	C3-C4-C5-C6
3	A	503	KNA	O2-C1-C2-C3
3	A	503	KNA	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	KNA	9	0
2	B	501	GFV	1	0
2	A	501	GFV	1	0
3	A	503	KNA	1	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

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	255/271 (94%)	0.72	31 (12%)	8 9	24, 39, 77, 105	0
1	B	263/271 (97%)	0.94	45 (17%)	4 4	24, 41, 94, 133	0
All	All	518/542 (95%)	0.83	76 (14%)	6 6	24, 40, 89, 133	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	465	LEU	7.4
1	B	476	LEU	7.1
1	B	268	THR	6.4
1	A	476	LEU	6.1
1	B	267	ILE	5.6
1	A	241	THR	5.6
1	A	242	THR	5.1
1	B	452	LEU	5.1
1	B	238	THR	5.0
1	B	266	HIS	4.7
1	B	464	SER	4.6
1	A	240	LYS	4.1
1	B	474	LYS	4.0
1	B	242	THR	3.9
1	A	256	MET	3.9
1	B	461	THR	3.9
1	B	363	PHE	3.9
1	A	258	GLY	3.8
1	B	440	THR	3.7
1	B	239	GLY	3.6
1	B	241	THR	3.6
1	B	473	TYR	3.5
1	B	456	ILE	3.3
1	B	462	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	359	PRO	3.2
1	A	354	LYS	3.1
1	A	243	ASP	3.1
1	B	453	LEU	3.1
1	A	336	LYS	3.0
1	B	457	LYS	3.0
1	B	455	VAL	3.0
1	A	257	MET	3.0
1	B	276	GLU	3.0
1	A	255	LEU	2.9
1	A	277	VAL	2.9
1	B	228	LEU	2.9
1	A	363	PHE	2.9
1	B	209	ALA	2.8
1	B	244	LYS	2.8
1	B	360	PHE	2.8
1	B	454	GLN	2.8
1	B	240	LYS	2.8
1	A	360	PHE	2.7
1	B	262	ILE	2.6
1	A	239	GLY	2.6
1	B	357	ARG	2.6
1	B	463	MET	2.6
1	B	260	ASP	2.6
1	A	359	PRO	2.5
1	B	475	ASP	2.5
1	B	256	MET	2.5
1	B	264	PHE	2.4
1	A	439	MET	2.4
1	B	450	VAL	2.4
1	B	277	VAL	2.4
1	A	358	LYS	2.4
1	A	440	THR	2.4
1	B	236	ILE	2.4
1	B	460	GLU	2.4
1	A	464	SER	2.4
1	A	282	PHE	2.3
1	A	401	LEU	2.3
1	A	427	GLU	2.3
1	B	466	HIS	2.3
1	B	459	THR	2.2
1	A	260	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	451	GLN	2.2
1	A	253	ASN	2.2
1	B	208	SER	2.2
1	A	357	ARG	2.1
1	B	458	LYS	2.1
1	A	452	LEU	2.1
1	A	469	LEU	2.1
1	A	402	ASN	2.0
1	A	362	ASP	2.0
1	A	443	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

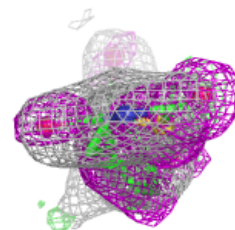
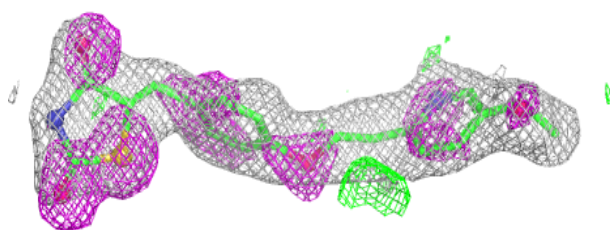
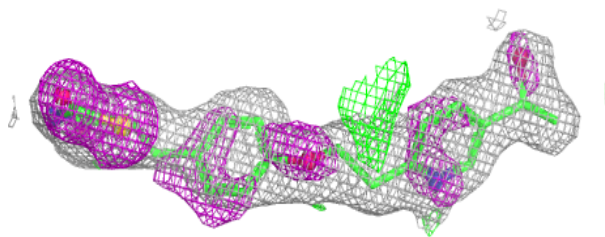
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	KNA	A	503	11/11	0.75	0.20	62,65,75,77	0
3	KNA	A	502	11/11	0.77	0.16	39,51,69,75	0
2	GFV	B	501	26/26	0.81	0.13	30,30,30,30	0
2	GFV	A	501	26/26	0.87	0.12	30,30,30,30	0

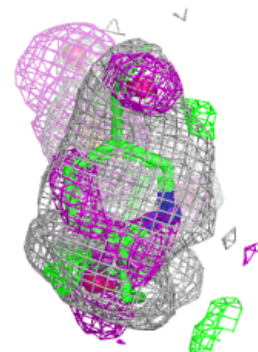
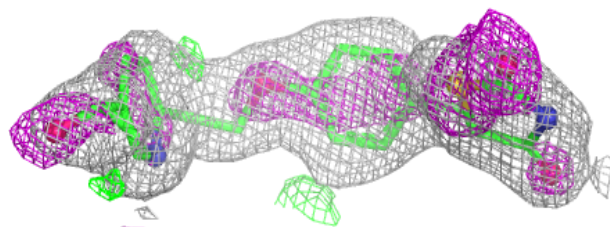
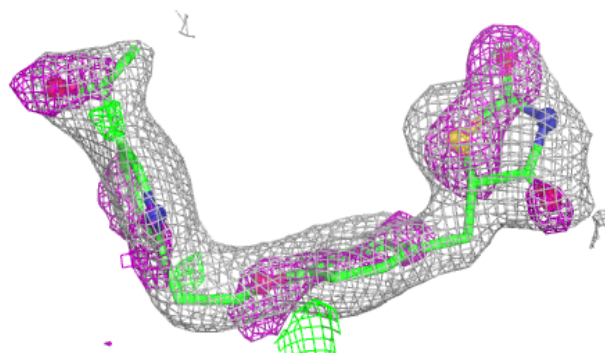
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GFV B 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GFV A 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.