WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 08:18 AM EST

PDB ID	:	4EMA
Title	:	Human peroxisome proliferator-activated receptor gamma in complex with rosiglitazone
Authors	:	Liberato, M.V.; Nascimento, A.S.; Polikarpov, I.
Deposited on	:	2012-04-11
Resolution	:	2.54 Å(reported)

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

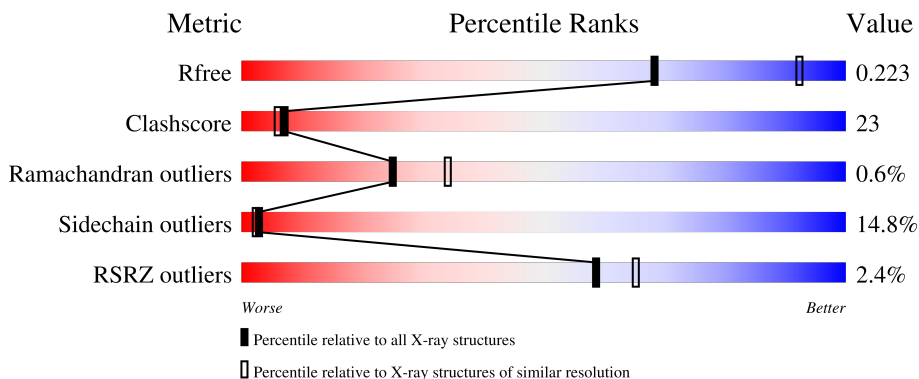|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.54 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	Percentile Ranks	Value
Rfree		0.223
Clashscore		23
Ramachandran outliers		0.6%
Sidechain outliers		14.8%
RSRZ outliers		2.4%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 <=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	275	3% 61% 26% 6% 7%
1	B	275	2% 49% 30% 9% 11%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4102 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	256	Total	C	N	O	S	1	0	0
			2049	1322	332	385	10			
1	B	244	Total	C	N	O	S	6	0	0
			1949	1258	317	364	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	GLY	-	expression tag	UNP P37231
A	204	SER	-	expression tag	UNP P37231
A	205	HIS	-	expression tag	UNP P37231
A	206	MET	-	expression tag	UNP P37231
B	203	GLY	-	expression tag	UNP P37231
B	204	SER	-	expression tag	UNP P37231
B	205	HIS	-	expression tag	UNP P37231
B	206	MET	-	expression tag	UNP P37231

- Molecule 2 is 2,4-THIAZOLIDIINEDIONE, 5-[[4-[2-(METHYL-2-PYRIDINYLAMINO)ET HOXY]PHENYL]METHYL]-(9CL) (three-letter code: BRL) (formula: $C_{18}H_{19}N_3O_3S$).
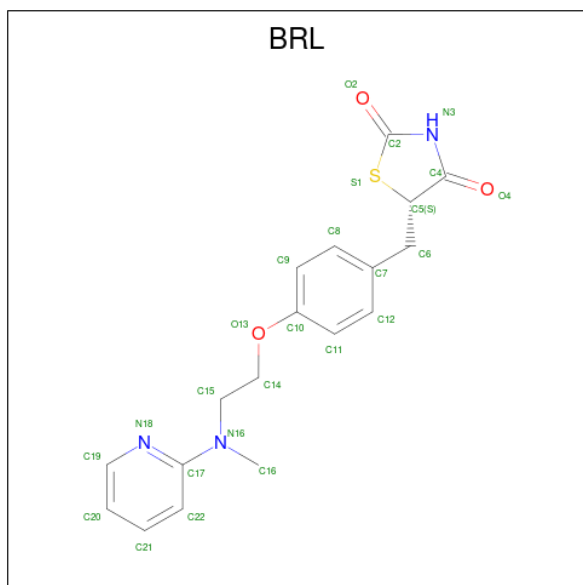
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	25	18	3	3	1	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	43	43	43	0	0
			Total	O		
3	B	36	36	36	0	0

3 Residue-property plots ⓘ

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

Chain A:

• Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:
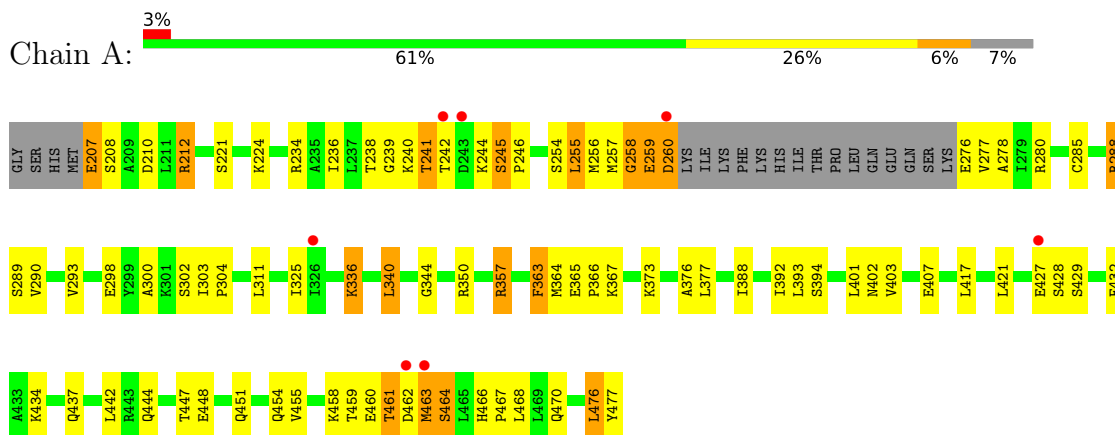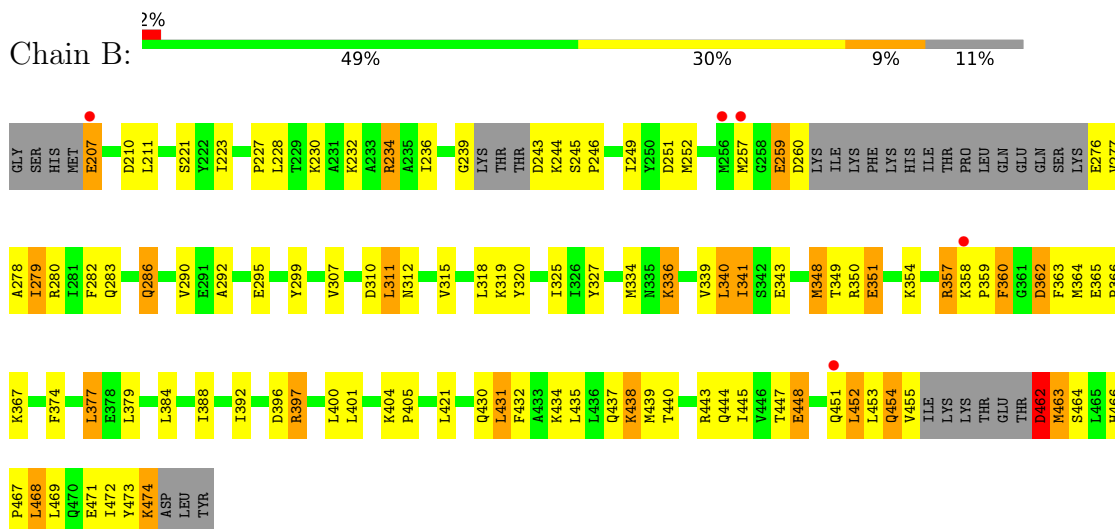
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	90.51Å 61.96Å 117.60Å 90.00° 100.70° 90.00°	Depositor
Resolution (Å)	28.89 – 2.54 28.89 – 2.54	Depositor EDS
% Data completeness (in resolution range)	98.2 (28.89-2.54) 98.1 (28.89-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.180 , 0.225 0.179 , 0.223	Depositor DCC
R_{free} test set	1071 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 72.0	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4102	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BRL

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	0.51	0/2083	0.73	0/2808
1	B	0.53	0/1980	0.80	2/2666 (0.1%)
All	All	0.52	0/4063	0.76	2/5474 (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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	239	GLY	N-CA-C	-7.15	95.23	113.10
1	B	207	GLU	CB-CA-C	6.82	124.04	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	462	ASP	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	2049	0	2098	73	0
1	B	1949	0	1988	113	0
2	A	25	0	19	2	0
3	A	43	0	0	0	0
3	B	36	0	0	5	0
All	All	4102	0	4105	184	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 23.

All (184) 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:462:ASP:OD1	1:B:463:MET:HB3	1.33	1.25
1:B:454:GLN:HB2	1:B:455:VAL:HB	1.27	1.15
1:B:468:LEU:O	1:B:471:GLU:HB2	1.58	1.03
1:B:454:GLN:CB	1:B:455:VAL:HB	1.90	1.00
1:B:463:MET:O	1:B:463:MET:HG3	1.59	0.99
1:A:460:GLU:HB3	1:A:463:MET:HG2	1.46	0.97
1:B:451:GLN:HG3	3:B:535:HOH:O	1.68	0.92
1:B:453:LEU:HD12	1:B:474:LYS:NZ	1.85	0.92
1:A:460:GLU:HB3	1:A:463:MET:CG	2.01	0.89
1:B:466:HIS:HD2	1:B:468:LEU:H	1.20	0.87
1:B:277:VAL:HG23	1:B:280:ARG:HH21	1.42	0.85
1:A:241:THR:OG1	1:A:244:LYS:HB2	1.77	0.84
1:A:357:ARG:CG	1:A:357:ARG:HH11	1.91	0.83
1:B:453:LEU:CD1	1:B:474:LYS:HZ1	1.91	0.82
1:B:228:LEU:HD12	1:B:232:LYS:HD2	1.61	0.81
1:B:278:ALA:HB1	1:B:360:PHE:CD2	2.17	0.80
1:B:454:GLN:HA	1:B:455:VAL:HG23	1.61	0.80
1:B:466:HIS:CD2	1:B:468:LEU:H	1.99	0.79
1:B:453:LEU:CD1	1:B:474:LYS:NZ	2.45	0.78
1:A:444:GLN:O	1:A:448:GLU:HG3	1.83	0.77
1:B:350:ARG:O	1:B:354:LYS:HG3	1.84	0.77
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.64	0.77
1:A:357:ARG:HH11	1:A:357:ARG:HG3	1.49	0.76
1:B:278:ALA:HB1	1:B:360:PHE:HD2	1.52	0.74
1:B:360:PHE:C	1:B:362:ASP:H	1.90	0.74
1:B:466:HIS:HD2	1:B:468:LEU:N	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLN:HA	1:B:455:VAL:CG2	2.18	0.73
1:B:430:GLN:O	1:B:434:LYS:HG3	1.90	0.72
1:A:276:GLU:HG3	1:A:280:ARG:NH1	2.05	0.72
1:B:453:LEU:HD12	1:B:474:LYS:HZ3	1.55	0.72
1:B:454:GLN:CA	1:B:455:VAL:HB	2.20	0.71
1:B:364:MET:HE2	1:B:367:LYS:HG3	1.71	0.71
1:A:285:CYS:HG	1:A:363:PHE:HZ	1.38	0.70
1:B:444:GLN:O	1:B:448:GLU:HG2	1.91	0.70
1:B:462:ASP:CG	1:B:463:MET:HB3	2.11	0.70
1:B:207:GLU:O	1:B:211:LEU:HG	1.93	0.69
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.58	0.69
1:A:241:THR:HG21	1:A:244:LYS:CE	2.23	0.69
1:A:403:VAL:CG1	1:A:407:GLU:OE2	2.41	0.69
1:A:455:VAL:O	1:A:459:THR:HB	1.95	0.67
1:B:462:ASP:OD1	1:B:462:ASP:C	2.34	0.67
1:A:241:THR:CB	1:A:244:LYS:HB2	2.26	0.66
1:B:454:GLN:HB2	1:B:455:VAL:CB	2.17	0.65
1:A:461:THR:O	1:A:462:ASP:OD1	2.15	0.65
1:B:360:PHE:O	1:B:362:ASP:N	2.30	0.64
1:B:360:PHE:N	1:B:360:PHE:HD1	1.95	0.64
1:A:212:ARG:HG3	1:A:212:ARG:NH1	2.12	0.63
1:B:360:PHE:N	1:B:360:PHE:CD1	2.65	0.62
1:A:300:ALA:HA	1:A:303:ILE:HD12	1.81	0.61
1:A:277:VAL:HG23	1:A:278:ALA:H	1.64	0.61
1:A:255:LEU:HD12	1:A:255:LEU:O	2.00	0.61
1:B:299:TYR:HE2	1:B:388:ILE:HG22	1.66	0.61
1:B:421:LEU:HD22	1:B:431:LEU:HD13	1.83	0.60
1:A:241:THR:OG1	1:A:244:LYS:HD2	2.02	0.60
1:A:460:GLU:HB3	1:A:463:MET:HG3	1.83	0.60
1:B:360:PHE:C	1:B:362:ASP:N	2.56	0.59
1:B:454:GLN:CA	1:B:455:VAL:CB	2.81	0.59
1:B:327:TYR:CE1	1:B:367:LYS:HE3	2.38	0.59
1:B:453:LEU:HD12	1:B:474:LYS:HZ1	1.49	0.58
1:A:373:LYS:NZ	1:B:396:ASP:HB3	2.19	0.57
1:A:241:THR:HG1	1:A:244:LYS:HB2	1.69	0.57
1:A:276:GLU:CG	1:A:280:ARG:NH1	2.67	0.57
1:B:334:MET:HG3	1:B:339:VAL:HG23	1.87	0.57
1:B:341:ILE:CD1	1:B:348:MET:HE2	2.35	0.57
1:B:360:PHE:O	1:B:363:PHE:HD2	1.87	0.57
1:A:357:ARG:NH2	1:A:460:GLU:OE2	2.29	0.56
1:B:454:GLN:HA	1:B:455:VAL:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:LEU:O	1:A:477:TYR:HB2	2.05	0.56
1:B:364:MET:HE2	1:B:367:LYS:CG	2.36	0.56
1:B:249:ILE:O	1:B:349:THR:HG23	2.06	0.55
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.41	0.55
1:A:241:THR:HG21	1:A:244:LYS:CD	2.37	0.55
1:B:310:ASP:OD1	1:B:312:ASN:ND2	2.36	0.55
1:B:359:PRO:O	1:B:362:ASP:HB2	2.07	0.55
1:B:236:ILE:CG2	1:B:246:PRO:HG3	2.37	0.54
1:A:238:THR:OG1	1:A:240:LYS:HE3	2.07	0.54
1:B:341:ILE:HD12	1:B:348:MET:CE	2.37	0.54
1:B:365:GLU:HB3	1:B:366:PRO:HD3	1.89	0.54
1:B:278:ALA:CB	1:B:360:PHE:CD2	2.89	0.54
1:B:341:ILE:HD12	1:B:348:MET:HE2	1.89	0.53
1:B:276:GLU:HG3	1:B:276:GLU:O	2.06	0.53
1:A:403:VAL:HG12	1:A:407:GLU:OE2	2.09	0.53
1:A:236:ILE:CG2	1:A:246:PRO:HG3	2.40	0.52
1:A:340:LEU:HG	1:A:344:GLY:HA2	1.91	0.52
1:B:327:TYR:CZ	1:B:367:LYS:HE3	2.44	0.52
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.22	0.52
1:A:434:LYS:HA	1:A:437:GLN:HE21	1.76	0.51
1:A:239:GLY:C	1:A:241:THR:H	2.13	0.50
1:B:464:SER:C	3:B:531:HOH:O	2.49	0.50
1:A:367:LYS:H	1:A:367:LYS:CD	2.25	0.50
1:A:277:VAL:HG23	1:A:278:ALA:N	2.26	0.50
1:A:373:LYS:O	1:A:376:ALA:HB3	2.11	0.50
1:B:462:ASP:OD1	1:B:462:ASP:O	2.30	0.50
1:A:259:GLU:O	1:A:260:ASP:O	2.29	0.49
1:A:357:ARG:HH11	1:A:357:ARG:HG2	1.74	0.49
1:A:241:THR:HB	1:A:244:LYS:HB2	1.94	0.49
1:B:360:PHE:O	1:B:363:PHE:CD2	2.64	0.49
1:B:443:ARG:O	1:B:447:THR:HG23	2.12	0.49
1:B:259:GLU:HG2	1:B:259:GLU:O	2.13	0.49
1:A:357:ARG:CG	1:A:357:ARG:NH1	2.61	0.48
1:B:290:VAL:HG21	1:B:473:TYR:CE1	2.48	0.48
1:A:357:ARG:HG2	1:A:357:ARG:O	2.12	0.48
1:B:364:MET:HE2	1:B:367:LYS:CD	2.44	0.48
1:A:288:ARG:HA	1:A:288:ARG:HD2	1.62	0.48
1:B:236:ILE:HG22	1:B:236:ILE:O	2.12	0.48
1:A:259:GLU:OE1	1:A:259:GLU:HA	2.00	0.48
1:A:373:LYS:HZ3	1:B:396:ASP:HB3	1.78	0.48
1:A:224:LYS:HE2	1:A:298:GLU:OE2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ASP:HB3	3:B:526:HOH:O	2.12	0.48
1:B:357:ARG:HE	1:B:357:ARG:HB2	1.46	0.47
1:A:302:SER:O	1:A:304:PRO:HD3	2.13	0.47
1:B:276:GLU:O	1:B:276:GLU:CG	2.62	0.47
1:B:432:PHE:HB3	3:B:501:HOH:O	2.15	0.47
1:A:212:ARG:NE	1:A:212:ARG:HA	2.29	0.47
1:B:307:VAL:HG12	1:B:307:VAL:O	2.13	0.47
1:A:212:ARG:HH11	1:A:212:ARG:CG	2.26	0.47
1:A:365:GLU:N	1:A:366:PRO:CD	2.78	0.47
1:B:299:TYR:CE2	1:B:388:ILE:HG22	2.48	0.47
1:A:285:CYS:SG	1:A:363:PHE:HZ	2.37	0.46
1:A:421:LEU:CD1	1:A:432:PHE:HA	2.45	0.46
1:A:454:GLN:O	1:A:458:LYS:HG3	2.14	0.46
1:B:292:ALA:HA	1:B:295:GLU:HG3	1.97	0.46
1:A:325:ILE:HG12	1:A:388:ILE:HB	1.96	0.46
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.51	0.46
1:B:207:GLU:HB3	1:B:210:ASP:OD2	2.15	0.46
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.96	0.46
1:A:336:LYS:NZ	1:A:350:ARG:HH12	2.14	0.46
1:A:364:MET:SD	2:A:601:BRL:H11	2.56	0.46
1:B:454:GLN:HA	1:B:455:VAL:HB	1.93	0.46
1:A:476:LEU:O	1:A:477:TYR:CB	2.65	0.45
1:B:374:PHE:O	1:B:377:LEU:HB2	2.15	0.45
1:B:466:HIS:CD2	1:B:466:HIS:C	2.89	0.45
1:A:245:SER:HA	1:A:246:PRO:HD3	1.58	0.45
1:A:241:THR:HG21	1:A:244:LYS:HE3	1.99	0.45
1:B:466:HIS:CG	1:B:467:PRO:HD2	2.53	0.44
1:A:293:VAL:HG11	1:A:468:LEU:HD21	1.98	0.44
1:B:340:LEU:HD12	1:B:340:LEU:HA	1.83	0.44
1:B:453:LEU:N	1:B:453:LEU:HD23	2.31	0.44
1:B:469:LEU:HA	1:B:472:ILE:HD12	1.99	0.44
1:A:207:GLU:O	1:A:210:ASP:HB2	2.18	0.44
1:A:254:SER:O	1:A:258:GLY:N	2.50	0.44
1:A:365:GLU:N	1:A:366:PRO:HD2	2.33	0.44
1:B:334:MET:CG	1:B:339:VAL:HG23	2.47	0.44
1:A:462:ASP:O	1:A:464:SER:N	2.51	0.43
1:B:365:GLU:N	1:B:366:PRO:CD	2.81	0.43
1:B:364:MET:CE	1:B:367:LYS:HE2	2.48	0.43
1:A:239:GLY:C	1:A:241:THR:N	2.72	0.43
1:A:417:LEU:HD23	1:A:432:PHE:HE1	1.82	0.43
1:B:404:LYS:HB3	1:B:405:PRO:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:PHE:CE1	1:B:364:MET:HG2	2.54	0.43
1:B:351:GLU:OE1	1:B:354:LYS:HD3	2.18	0.43
1:B:374:PHE:HD1	1:B:438:LYS:HG2	1.84	0.43
1:A:276:GLU:HG2	1:A:280:ARG:HH12	1.84	0.42
1:B:444:GLN:O	1:B:448:GLU:CG	2.65	0.42
1:A:367:LYS:H	1:A:367:LYS:HD2	1.84	0.42
1:A:467:PRO:O	1:A:470:GLN:HB2	2.19	0.42
1:B:260:ASP:OD1	1:B:260:ASP:C	2.58	0.42
1:B:279:ILE:HD12	1:B:463:MET:HA	2.01	0.42
1:B:379:LEU:HD11	1:B:435:LEU:HD13	2.00	0.42
1:B:452:LEU:HD23	1:B:452:LEU:HA	1.57	0.42
1:B:336:LYS:O	1:B:350:ARG:HD2	2.19	0.42
1:B:365:GLU:N	1:B:366:PRO:HD2	2.34	0.42
1:B:448:GLU:HG2	1:B:448:GLU:H	1.57	0.42
1:B:227:PRO:O	1:B:232:LYS:CE	2.67	0.42
1:B:282:PHE:C	1:B:282:PHE:CD1	2.92	0.42
1:B:452:LEU:C	1:B:453:LEU:HD23	2.39	0.42
1:B:311:LEU:HD23	1:B:315:VAL:HG23	2.00	0.42
1:B:283:GLN:O	1:B:286:GLN:HB2	2.20	0.41
1:A:289:SER:OG	2:A:601:BRL:H5	2.20	0.41
1:A:392:ILE:HG22	1:A:393:LEU:HD22	2.01	0.41
1:B:468:LEU:HA	1:B:468:LEU:HD12	1.76	0.41
1:B:318:LEU:O	1:B:319:LYS:C	2.58	0.41
1:B:230:LYS:O	1:B:234:ARG:HB2	2.20	0.41
1:A:276:GLU:CG	1:A:280:ARG:HH12	2.32	0.41
1:B:445:ILE:HD13	1:B:445:ILE:HA	1.84	0.41
1:B:286:GLN:OE1	1:B:286:GLN:CA	2.68	0.41
1:B:320:TYR:HB2	1:B:397:ARG:CG	2.51	0.41
1:B:430:GLN:NE2	3:B:501:HOH:O	2.54	0.41
1:B:437:GLN:O	1:B:440:THR:HB	2.21	0.41
1:B:251:ASP:OD1	1:B:251:ASP:C	2.59	0.40
1:B:466:HIS:CD2	1:B:467:PRO:HD2	2.56	0.40
1:B:358:LYS:HG3	1:B:359:PRO:HA	2.02	0.40
1:B:364:MET:CE	1:B:364:MET:HA	2.51	0.40
1:B:223:ILE:HD13	1:B:223:ILE:HA	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	252/275 (92%)	238 (94%)	12 (5%)	2 (1%)	19	27
1	B	236/275 (86%)	218 (92%)	17 (7%)	1 (0%)	34	46
All	All	488/550 (89%)	456 (93%)	29 (6%)	3 (1%)	25	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	336	LYS
1	A	463	MET
1	A	258	GLY

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	229/247 (93%)	197 (86%)	32 (14%)	3	3
1	B	217/247 (88%)	183 (84%)	34 (16%)	2	2
All	All	446/494 (90%)	380 (85%)	66 (15%)	3	2

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	GLU
1	A	208	SER
1	A	212	ARG

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Mol	Chain	Res	Type
1	A	221	SER
1	A	234	ARG
1	A	241	THR
1	A	242	THR
1	A	245	SER
1	A	255	LEU
1	A	256	MET
1	A	257	MET
1	A	259	GLU
1	A	260	ASP
1	A	288	ARG
1	A	311	LEU
1	A	336	LYS
1	A	340	LEU
1	A	357	ARG
1	A	363	PHE
1	A	377	LEU
1	A	394	SER
1	A	401	LEU
1	A	402	ASN
1	A	427	GLU
1	A	428	SER
1	A	429	SER
1	A	442	LEU
1	A	447	THR
1	A	451	GLN
1	A	461	THR
1	A	464	SER
1	A	476	LEU
1	B	221	SER
1	B	234	ARG
1	B	243	ASP
1	B	244	LYS
1	B	245	SER
1	B	252	MET
1	B	257	MET
1	B	259	GLU
1	B	279	ILE
1	B	286	GLN
1	B	311	LEU
1	B	340	LEU
1	B	341	ILE

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Mol	Chain	Res	Type
1	B	343	GLU
1	B	348	MET
1	B	351	GLU
1	B	357	ARG
1	B	360	PHE
1	B	362	ASP
1	B	377	LEU
1	B	384	LEU
1	B	397	ARG
1	B	400	LEU
1	B	401	LEU
1	B	431	LEU
1	B	438	LYS
1	B	439	MET
1	B	448	GLU
1	B	452	LEU
1	B	454	GLN
1	B	462	ASP
1	B	463	MET
1	B	468	LEU
1	B	474	LYS

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

Mol	Chain	Res	Type
1	A	286	GLN
1	A	314	GLN
1	A	345	GLN
1	A	415	GLN
1	A	437	GLN
1	A	454	GLN
1	A	470	GLN
1	B	294	GLN
1	B	314	GLN
1	B	345	GLN
1	B	412	ASN
1	B	430	GLN
1	B	444	GLN
1	B	454	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 monosaccharides 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	BRL	A	601	-	27,27,27	2.84	7 (25%)	36,36,36	2.81	10 (27%)

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	BRL	A	601	-	-	2/14/26/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BRL	C2-S1	-12.80	1.65	1.76
2	A	601	BRL	C4-N3	-3.54	1.33	1.37
2	A	601	BRL	C2-N3	-3.39	1.32	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	BRL	C5-C4	-2.21	1.51	1.52
2	A	601	BRL	O13-C14	-2.06	1.36	1.43
2	A	601	BRL	O13-C10	-2.05	1.32	1.37
2	A	601	BRL	C17-N16	-2.03	1.31	1.37

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	BRL	C4-C5-S1	-8.15	98.93	105.90
2	A	601	BRL	C5-S1-C2	8.08	97.21	92.86
2	A	601	BRL	C5-C4-N3	6.03	117.25	112.01
2	A	601	BRL	C4-N3-C2	-4.40	115.27	118.24
2	A	601	BRL	C19-N18-C17	4.17	122.37	116.86
2	A	601	BRL	C15-N16-C17	-3.52	117.24	120.94
2	A	601	BRL	N18-C17-N16	3.50	120.83	116.39
2	A	601	BRL	C16-N16-C15	3.05	123.73	115.42
2	A	601	BRL	O4-C4-N3	-2.90	121.44	124.94
2	A	601	BRL	C14-O13-C10	-2.83	110.53	117.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BRL	C9-C10-O13-C14
2	A	601	BRL	C11-C10-O13-C14

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	BRL	2	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 then 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.

Ligand BRL A 601

Bond lengths

Bond angles

Torsions

Rings
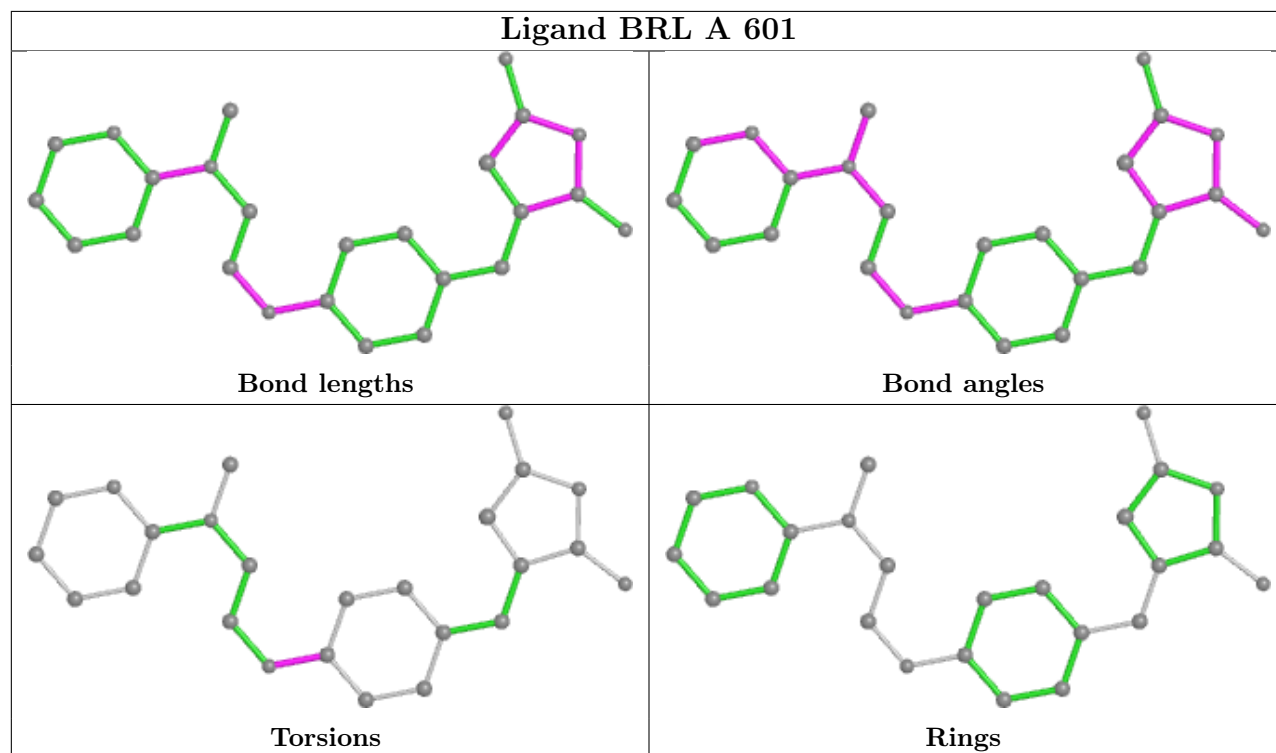
5.7 Other polymers (i)

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, 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(Å²)	Q<0.9
1	A	256/275 (93%)	-0.17	7 (2%)	54	61	31, 53, 89, 148	6 (2%)
1	B	244/275 (88%)	-0.12	5 (2%)	65	72	29, 59, 100, 134	11 (4%)
All	All	500/550 (90%)	-0.15	12 (2%)	59	65	29, 55, 97, 148	17 (3%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	451	GLN	3.7
1	A	242	THR	3.6
1	A	427	GLU	2.9
1	B	207	GLU	2.8
1	B	358	LYS	2.8
1	A	243	ASP	2.6
1	B	257	MET	2.5
1	A	462	ASP	2.5
1	A	463	MET	2.3
1	B	256	MET	2.3
1	A	260	ASP	2.1
1	A	326	ILE	2.1

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 ⓘ
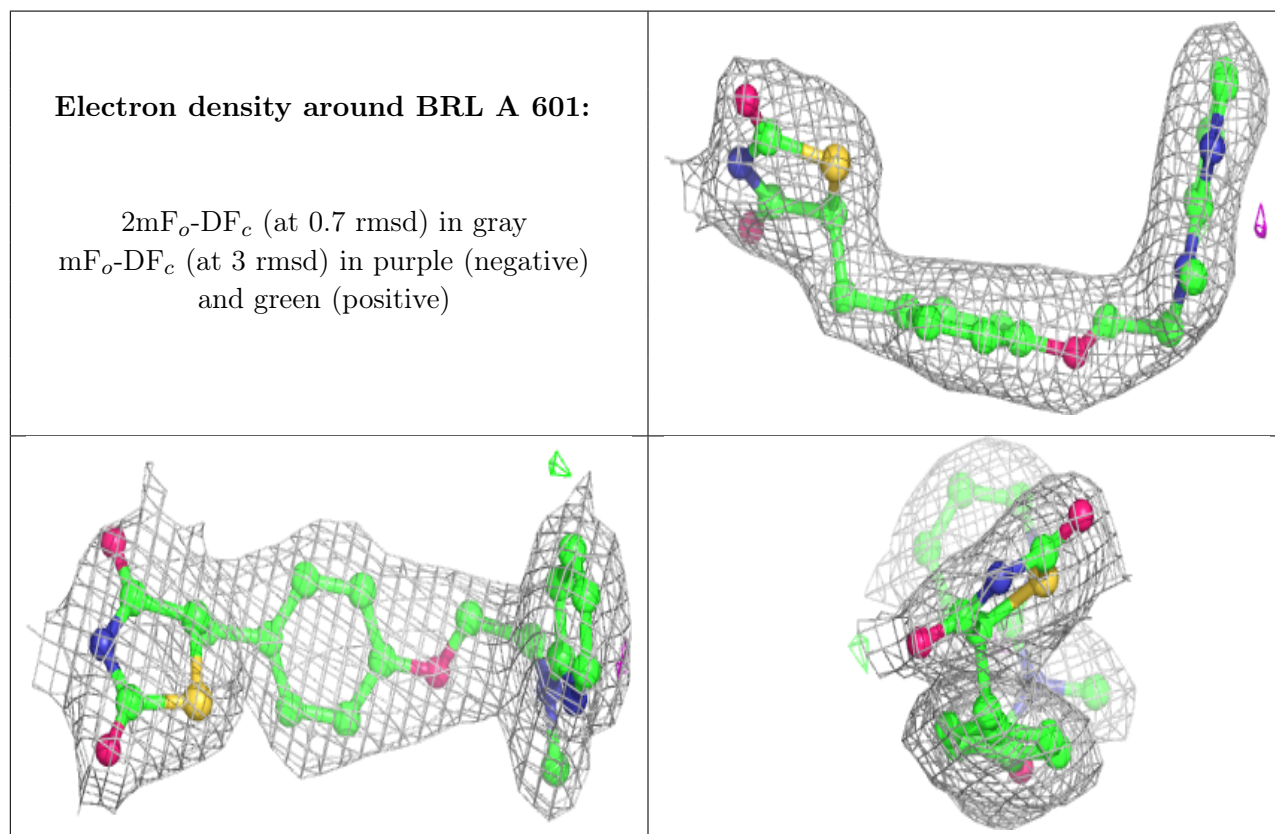
There are no monosaccharides in this entry.

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. 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(Å^2)	Q<0.9
2	BRL	A	601	25/25	0.95	0.14	52,64,84,85	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 BRL A 601:

$2\text{mF}_o\text{-DF}_c$ (at 0.7 rmsd) in gray
$\text{mF}_o\text{-DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)

6.5　Other polymers ⓘ

There are no such residues in this entry.