Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:51 AM GMT

PDB ID	:	3GBK
Title	:	Crystal Structure of Human PPAR-gamma Ligand Binding Domain Complexed with a Potent and Selective Agonist
Authors	:	Peng, Y.-H.; Lin, C.-H.; Hsieh, H.-P.; Wu, S.-Y.
Deposited on	:	2009-02-19
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

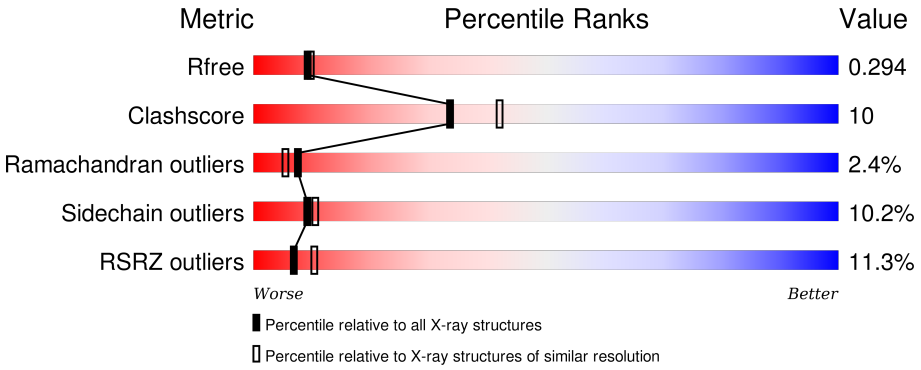
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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 <=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	8% 77% 18% 5%
1	B	271	14% 72% 23% 5%

2 Entry composition

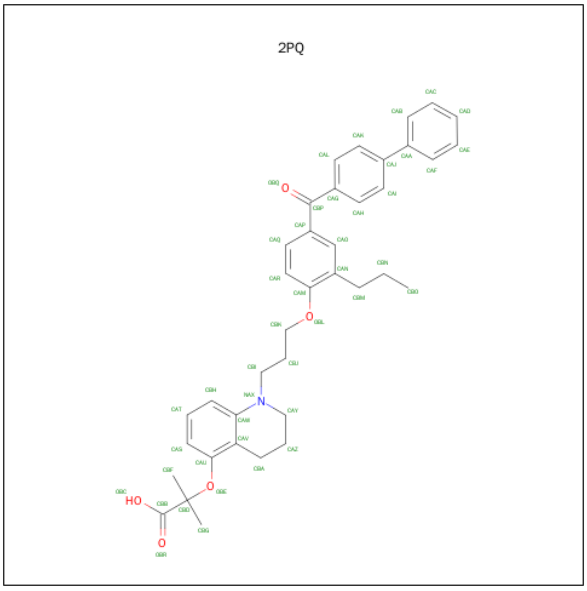
There are 3 unique types of molecules in this entry. The entry contains 4473 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	271	Total	C	N	O	S	0	0	0
			2178	1406	355	407	10			
1	B	271	Total	C	N	O	S	0	0	0
			2178	1406	355	407	10			

- Molecule 2 is 2-[(1-{3-[4-(BIPHENYL-4-YLCARBONYL)-2-PROPYLPHENOXY]PROPYL}-1,2,3,4-TETRAHYDROQUINOLIN-5-YL)OXY]-2-METHYLPROPANOIC ACID (three-letter code: 2PQ) (formula: $C_{38}H_{41}NO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			44	38	1	5		

- Molecule 3 is water.

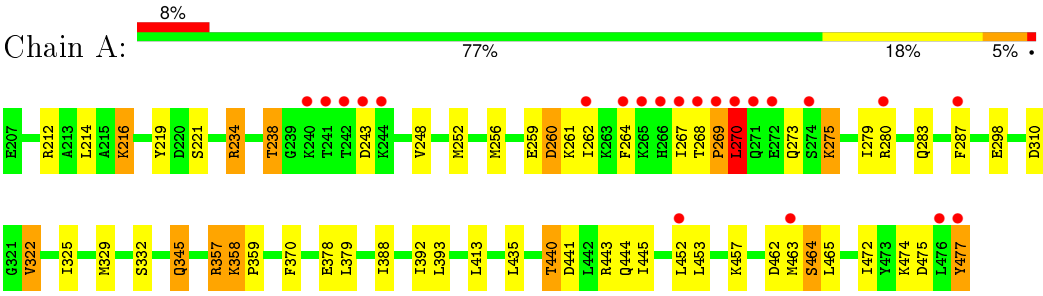
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0
3	B	39	Total O 39 39	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

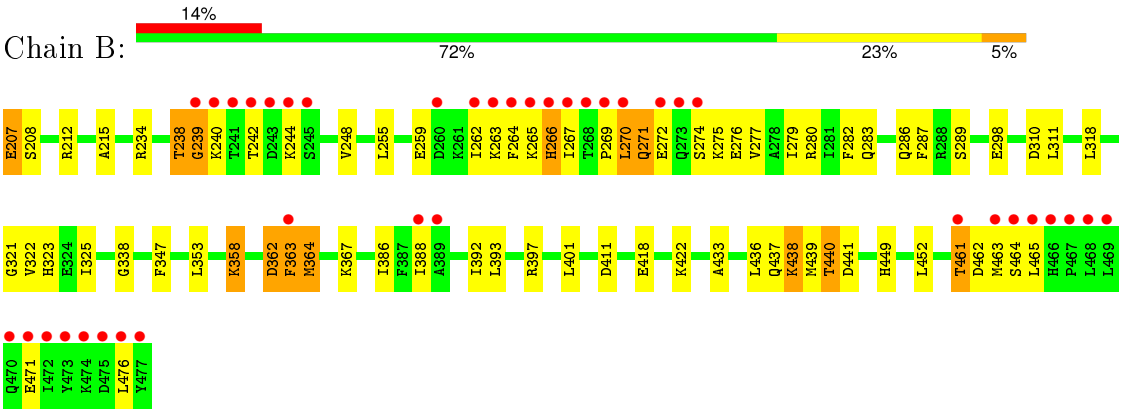
- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain A:



- Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.50Å 88.89Å 58.37Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	26.12 – 2.30 26.12 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (26.12-2.30) 97.9 (26.12-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.32 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.298 0.229 , 0.294	Depositor DCC
R_{free} test set	1279 reflections (5.34%)	DCC
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.1	EDS
Estimated twinning fraction	0.002 for l,k,-h 0.034 for h,-k,-l 0.026 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 25251 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4473	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 2PQ

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	0.93	0/2216	0.87	2/2985 (0.1%)
1	B	0.91	1/2216 (0.0%)	0.91	2/2985 (0.1%)
All	All	0.92	1/4432 (0.0%)	0.89	4/5970 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	298	GLU	CG-CD	5.42	1.60	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	212	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	318	LEU	CD1-CG-CD2	5.41	126.73	110.50
1	B	397	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	270	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

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	2178	0	2241	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2178	0	2241	46	0
2	A	44	0	40	5	0
3	A	34	0	0	7	0
3	B	39	0	0	6	0
All	All	4473	0	4522	91	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 10.

All (91) 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:207:GLU:HG3	3:B:38:HOH:O	1.50	1.09
1:B:270:LEU:HB2	3:B:56:HOH:O	1.55	1.05
1:A:345:GLN:HG3	3:A:22:HOH:O	1.62	1.00
1:A:440:THR:O	1:A:444:GLN:HG3	1.75	0.87
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.59	0.85
1:A:444:GLN:HB3	3:A:51:HOH:O	1.81	0.80
1:A:269:PRO:HB2	1:A:287:PHE:CZ	2.20	0.77
1:A:444:GLN:CB	3:A:51:HOH:O	2.34	0.76
1:A:477:TYR:O	1:A:477:TYR:CD1	2.38	0.76
1:A:259:GLU:OE2	1:A:280:ARG:NH2	2.20	0.74
1:B:461:THR:HA	3:B:58:HOH:O	1.88	0.73
1:A:463:MET:HG3	1:A:464:SER:H	1.55	0.72
1:A:279:ILE:O	1:A:283:GLN:HG3	1.91	0.70
1:B:275:LYS:HG3	1:B:276:GLU:H	1.57	0.69
1:A:234:ARG:O	1:A:238:THR:HB	1.94	0.68
1:B:270:LEU:HD23	1:B:287:PHE:CD2	2.31	0.65
1:A:256:MET:O	1:A:260:ASP:HB2	1.96	0.64
1:A:268:THR:O	1:A:270:LEU:N	2.31	0.63
1:A:269:PRO:HB2	1:A:287:PHE:HZ	1.64	0.61
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.36	0.59
1:A:310:ASP:OD2	1:B:269:PRO:HD2	2.03	0.59
1:B:321:GLY:O	1:B:325:ILE:HD12	2.02	0.58
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.86	0.58
1:B:259:GLU:HG3	1:B:280:ARG:HH22	1.68	0.58
1:B:363:PHE:CE1	1:B:449:HIS:CE1	2.91	0.57
1:B:353:LEU:HD22	1:B:364:MET:HG2	1.86	0.57
1:B:270:LEU:O	1:B:271:GLN:HB2	2.03	0.57
1:B:363:PHE:CZ	1:B:452:LEU:HB3	2.38	0.57
1:B:358:LYS:O	1:B:362:ASP:OD2	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:LYS:HE3	3:B:65:HOH:O	2.04	0.57
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.87	0.56
1:B:270:LEU:CB	3:B:56:HOH:O	2.29	0.56
1:A:474:LYS:HE2	1:A:475:ASP:OD2	2.05	0.55
1:A:259:GLU:CD	2:A:1385:2PQ:HAD	2.27	0.55
1:A:477:TYR:O	1:A:477:TYR:HD1	1.86	0.55
1:B:275:LYS:HE3	1:B:462:ASP:HB2	1.87	0.55
1:B:437:GLN:O	1:B:440:THR:HG23	2.07	0.54
1:B:279:ILE:O	1:B:283:GLN:HG3	2.07	0.54
1:A:216:LYS:CE	3:A:61:HOH:O	2.56	0.53
1:A:322:VAL:HG11	1:A:472:ILE:HD13	1.90	0.53
1:B:263:LYS:HD3	1:B:263:LYS:O	2.09	0.52
1:B:364:MET:O	1:B:367:LYS:HB2	2.10	0.51
1:A:392:ILE:HG22	1:A:393:LEU:HD22	1.92	0.51
1:A:259:GLU:HG2	2:A:1385:2PQ:HAD	1.91	0.50
1:A:357:ARG:HB2	1:A:357:ARG:HH11	1.75	0.50
1:A:275:LYS:HG2	1:A:279:ILE:HG21	1.94	0.50
1:A:318:LEU:O	1:A:322:VAL:HB	2.11	0.50
1:A:216:LYS:HE3	3:A:61:HOH:O	2.12	0.50
1:B:242:THR:O	1:B:242:THR:HG23	2.12	0.50
1:B:310:ASP:OD2	1:B:401:LEU:HD12	2.12	0.50
1:B:271:GLN:HG2	1:B:272:GLU:H	1.77	0.49
1:A:259:GLU:O	1:A:261:LYS:N	2.46	0.48
1:A:319:LYS:NZ	1:A:474:LYS:O	2.34	0.48
1:A:259:GLU:C	1:A:261:LYS:H	2.17	0.48
1:A:457:LYS:HG2	1:A:463:MET:SD	2.53	0.48
1:B:275:LYS:HG3	1:B:276:GLU:N	2.25	0.47
1:B:238:THR:HB	1:B:239:GLY:H	1.25	0.47
1:B:392:ILE:HG22	1:B:393:LEU:HD22	1.97	0.46
1:A:329:MET:O	1:A:332:SER:HB2	2.14	0.46
1:A:259:GLU:CG	2:A:1385:2PQ:HAD	2.46	0.46
2:A:1385:2PQ:HBJ	2:A:1385:2PQ:HAY	1.71	0.45
1:B:259:GLU:CG	1:B:280:ARG:HH22	2.29	0.45
1:B:436:LEU:O	1:B:439:MET:HB2	2.16	0.45
1:B:418:GLU:HG2	1:B:422:LYS:HE2	1.99	0.45
1:B:255:LEU:CD2	1:B:277:VAL:CG1	2.95	0.44
1:A:310:ASP:OD2	1:B:269:PRO:CD	2.64	0.44
2:A:1385:2PQ:HBM	2:A:1385:2PQ:HBIA	1.98	0.44
1:B:438:LYS:HA	1:B:438:LYS:HD2	1.71	0.44
1:B:433:ALA:O	1:B:437:GLN:HG3	2.18	0.44
1:B:325:ILE:HD11	1:B:392:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:MET:SD	1:B:465:LEU:HD13	2.57	0.44
1:B:255:LEU:CD2	1:B:277:VAL:HG13	2.48	0.44
1:B:276:GLU:O	1:B:280:ARG:HG3	2.19	0.43
1:A:219:TYR:CD2	3:A:61:HOH:O	2.57	0.43
1:B:363:PHE:HE1	1:B:449:HIS:CE1	2.36	0.43
1:A:275:LYS:HB2	3:A:45:HOH:O	2.18	0.42
1:B:270:LEU:HD12	3:B:17:HOH:O	2.18	0.42
1:A:320:TYR:HE2	1:A:477:TYR:H	1.68	0.42
1:A:214:LEU:HD21	1:A:413:LEU:HD23	2.01	0.42
1:B:255:LEU:HD21	1:B:277:VAL:HG13	2.02	0.42
1:A:358:LYS:HB3	1:A:359:PRO:HD3	2.03	0.41
1:B:282:PHE:O	1:B:286:GLN:HG3	2.21	0.41
1:A:259:GLU:C	1:A:261:LYS:N	2.73	0.41
1:B:388:ILE:HA	1:B:388:ILE:HD13	1.84	0.41
1:A:379:LEU:HD11	1:A:435:LEU:HD13	2.03	0.41
1:B:215:ALA:CB	1:B:386:ILE:HD11	2.51	0.41
1:A:463:MET:HG3	1:A:464:SER:N	2.29	0.41
1:A:212:ARG:HD2	1:A:212:ARG:HA	1.83	0.41
1:B:362:ASP:OD1	1:B:452:LEU:HD21	2.22	0.40
1:B:265:LYS:HG3	1:B:266:HIS:H	1.86	0.40
1:A:345:GLN:HA	1:A:345:GLN:HE21	1.86	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	269/271 (99%)	248 (92%)	14 (5%)	7 (3%)	7	4
1	B	269/271 (99%)	243 (90%)	20 (7%)	6 (2%)	8	6
All	All	538/542 (99%)	491 (91%)	34 (6%)	13 (2%)	7	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	ASP
1	A	269	PRO
1	A	464	SER
1	B	464	SER
1	A	358	LYS
1	B	267	ILE
1	B	271	GLN
1	A	243	ASP
1	B	274	SER
1	B	266	HIS
1	A	262	ILE
1	B	239	GLY
1	A	267	ILE

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	244/244 (100%)	220 (90%)	24 (10%)	10 11
1	B	244/244 (100%)	218 (89%)	26 (11%)	8 9
All	All	488/488 (100%)	438 (90%)	50 (10%)	9 10

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	216	LYS
1	A	221	SER
1	A	234	ARG
1	A	238	THR
1	A	248	VAL
1	A	252	MET
1	A	264	PHE
1	A	270	LEU
1	A	273	GLN
1	A	275	LYS

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Mol	Chain	Res	Type
1	A	298	GLU
1	A	318	LEU
1	A	322	VAL
1	A	345	GLN
1	A	357	ARG
1	A	378	GLU
1	A	440	THR
1	A	441	ASP
1	A	443	ARG
1	A	452	LEU
1	A	453	LEU
1	A	462	ASP
1	A	465	LEU
1	A	477	TYR
1	B	207	GLU
1	B	208	SER
1	B	234	ARG
1	B	238	THR
1	B	240	LYS
1	B	244	LYS
1	B	248	VAL
1	B	262	ILE
1	B	264	PHE
1	B	270	LEU
1	B	289	SER
1	B	311	LEU
1	B	318	LEU
1	B	322	VAL
1	B	323	HIS
1	B	358	LYS
1	B	362	ASP
1	B	363	PHE
1	B	364	MET
1	B	411	ASP
1	B	438	LYS
1	B	440	THR
1	B	441	ASP
1	B	461	THR
1	B	471	GLU
1	B	476	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	345	GLN
1	A	451	GLN
1	B	271	GLN
1	B	273	GLN
1	B	466	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	2PQ	A	1385	-	45,48,48	1.11	3 (6%)	60,67,67	1.28	7 (11%)

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	2PQ	A	1385	-	-	0/27/43/43	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1385	2PQ	CAA-CAJ	-3.82	1.39	1.49
2	A	1385	2PQ	CAP-CBP	2.09	1.53	1.49
2	A	1385	2PQ	CBA-CAV	2.10	1.55	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1385	2PQ	CAK-CAL-CAG	-2.40	117.98	120.76
2	A	1385	2PQ	CAH-CAI-CAJ	-2.16	117.98	121.14
2	A	1385	2PQ	CAH-CAG-CAL	2.05	121.64	118.60
2	A	1385	2PQ	CAF-CAA-CAB	2.16	121.63	117.55
2	A	1385	2PQ	CAI-CAJ-CAK	2.35	122.00	117.55
2	A	1385	2PQ	CBK-OBL-CAM	3.38	125.94	117.64
2	A	1385	2PQ	CBD-OBE-CAU	4.65	128.89	120.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1385	2PQ	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.35	22 (8%) 15 21	22, 36, 77, 101	0
1	B	271/271 (100%)	0.83	39 (14%) 3 5	20, 36, 97, 121	0
All	All	542/542 (100%)	0.59	61 (11%) 7 10	20, 36, 92, 121	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	477	TYR	18.0
1	B	476	LEU	15.4
1	B	465	LEU	13.8
1	B	472	ILE	10.9
1	A	271	GLN	8.9
1	A	267	ILE	8.3
1	B	468	LEU	8.3
1	B	241	THR	8.2
1	B	475	ASP	8.1
1	B	272	GLU	7.4
1	A	270	LEU	7.4
1	A	262	ILE	7.2
1	B	474	LYS	7.1
1	B	273	GLN	6.9
1	B	267	ILE	6.7
1	B	473	TYR	6.6
1	B	240	LYS	6.4
1	A	272	GLU	6.3
1	A	242	THR	6.0
1	B	269	PRO	6.0
1	B	464	SER	6.0
1	B	265	LYS	5.9
1	A	268	THR	5.9
1	A	477	TYR	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	463	MET	5.5
1	B	266	HIS	5.4
1	B	242	THR	5.2
1	B	243	ASP	5.2
1	B	467	PRO	5.2
1	B	270	LEU	4.6
1	A	264	PHE	4.6
1	B	262	ILE	4.5
1	B	239	GLY	4.3
1	B	264	PHE	4.1
1	A	244	LYS	4.1
1	B	469	LEU	4.1
1	B	274	SER	4.0
1	B	260	ASP	4.0
1	A	269	PRO	3.9
1	B	363	PHE	3.8
1	B	268	THR	3.8
1	A	274	SER	3.7
1	B	471	GLU	3.5
1	A	241	THR	3.4
1	A	463	MET	3.3
1	A	243	ASP	3.2
1	B	470	GLN	3.1
1	B	263	LYS	3.1
1	B	245	SER	3.1
1	B	244	LYS	3.0
1	A	266	HIS	2.9
1	B	389	ALA	2.8
1	A	452	LEU	2.8
1	B	466	HIS	2.7
1	A	265	LYS	2.6
1	A	287	PHE	2.6
1	A	240	LYS	2.5
1	A	476	LEU	2.3
1	B	461	THR	2.2
1	B	388	ILE	2.1
1	A	280	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, 95^{th} 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(Å^2)	Q<0.9
2	2PQ	A	1385	44/44	0.85	0.20	0.37	39,48,59,60	0

6.5 Other polymers (i)

There are no such residues in this entry.