



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 12:56 AM EST

PDB ID : 1YUC
Title : Human Nuclear Receptor Liver Receptor Homologue-1, LRH-1, Bound to Phospholipid and a Fragment of Human SHP
Authors : Ortlund, E.A.; Yoonkwang, L.; Solomon, I.H.; Hager, J.M.; Safi, R.; Choi, Y.; Guan, Z.; Tripathy, A.; Raetz, C.R.H.; McDonnell, D.P.; Moore, D.D.; Redinbo, M.R.
Deposited on : 2005-02-13
Resolution : 1.90 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

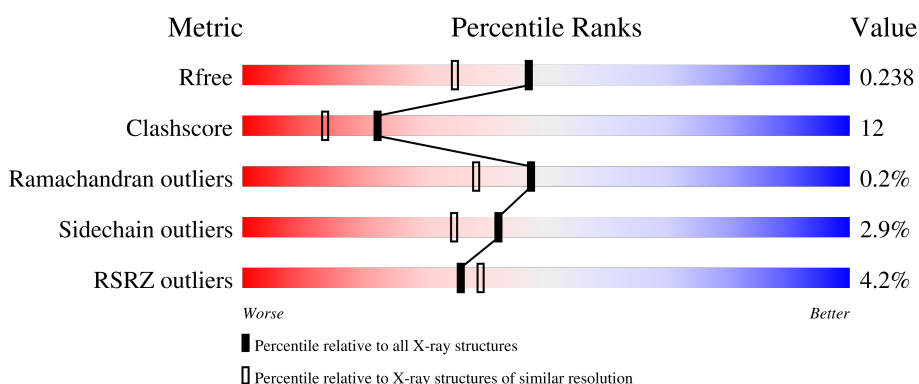
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	255	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 73%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 73% 20% • 6%</p>
1	B	255	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 72%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 72% 20% • 6%</p>
2	C	14	<div style="display: flex; align-items: center;"> <div style="width: 14%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">14% 79% 21%</p>
2	D	14	<div style="display: flex; align-items: center;"> <div style="width: 21%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">21% 64% 7% 7% 21%</p>

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
4	GOL	A	5001	-	X	-	-
4	GOL	B	5002	-	X	-	-
4	GOL	B	5003	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4443 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 Orphan nuclear receptor NR5A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	240	Total	C	N	O	S	9	0	0
			1948	1249	326	360	13			
1	B	240	Total	C	N	O	S	9	0	0
			1952	1252	327	360	13			

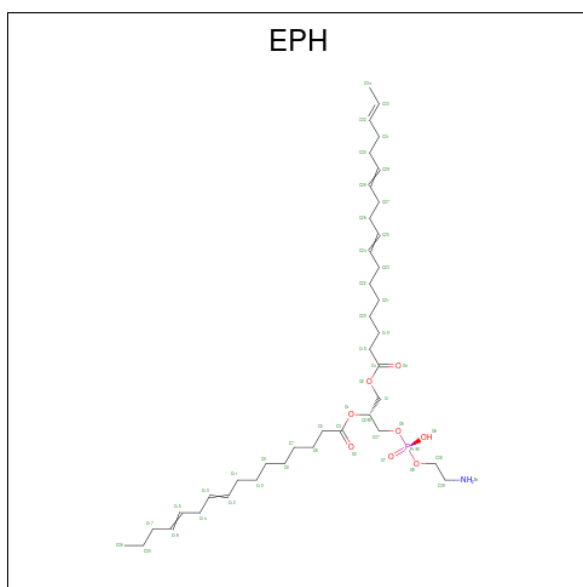
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	GLY	-	cloning artifact	UNP O00482
A	288	GLU	-	cloning artifact	UNP O00482
A	289	PHE	-	cloning artifact	UNP O00482
B	287	GLY	-	cloning artifact	UNP O00482
B	288	GLU	-	cloning artifact	UNP O00482
B	289	PHE	-	cloning artifact	UNP O00482

- Molecule 2 is a protein called Nuclear receptor 0B2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	14	Total	C	N	O	0	0	0
			102	65	17	20			
2	D	11	Total	C	N	O	0	0	0
			84	56	14	14			

- Molecule 3 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: C₃₉H₆₈NO₈P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	O			P
3	A	1	47	38	8	1	47	0
3	B	1	47	38	8	1	47	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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


- Molecule 5 is water.

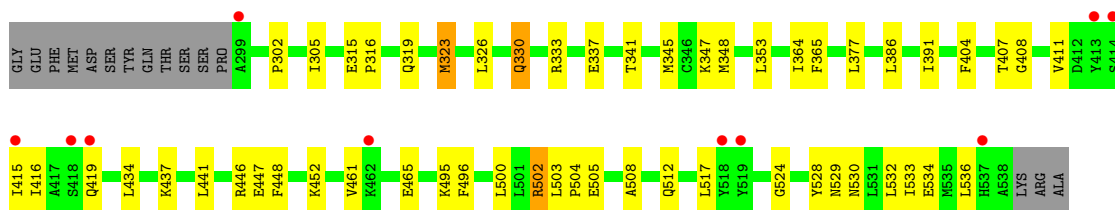
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	124	Total	O	0	0
			124	124		
5	B	110	Total	O	0	0
			110	110		
5	C	9	Total	O	0	0
			9	9		
5	D	2	Total	O	0	0
			2	2		

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.

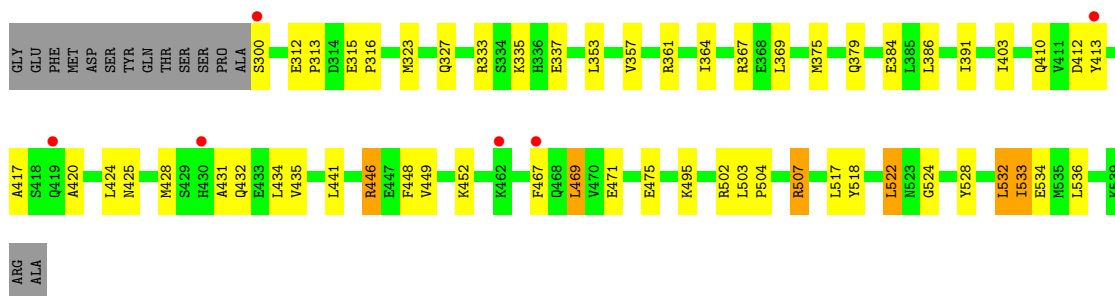
- Molecule 1: Orphan nuclear receptor NR5A2

Chain A: 




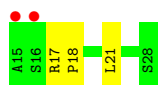
- Molecule 1: Orphan nuclear receptor NR5A2

Chain B: 



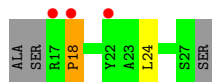
- Molecule 2: Nuclear receptor 0B2

Chain C: 



- Molecule 2: Nuclear receptor 0B2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.67Å 59.64Å 73.24Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	31.28 – 1.90 31.28 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (31.28-1.90) 97.0 (31.28-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 1.89Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.248 0.208 , 0.238	Depositor DCC
R_{free} test set	2137 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtrriage
Anisotropy	0.425	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4443	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.42% 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: GOL, EPH

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	0.32	0/1984	0.52	0/2680
1	B	0.31	0/1988	0.50	0/2684
2	C	0.35	0/103	0.54	0/138
2	D	0.32	0/85	0.49	0/115
All	All	0.32	0/4160	0.51	0/5617

There are no bond length outliers.

There are no bond angle outliers.

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	1948	0	1957	49	0
1	B	1952	0	1965	48	0
2	C	102	0	107	3	0
2	D	84	0	92	5	0
3	A	47	0	61	0	0
3	B	47	0	61	0	0
4	A	6	0	4	0	0
4	B	12	0	8	0	0
5	A	124	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	110	0	0	5	0
5	C	9	0	0	0	0
5	D	2	0	0	0	0
All	All	4443	0	4255	96	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 12.

All (96) 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:A:323:MET:HG2	1:A:407:THR:HB	1.44	0.99
1:A:391:ILE:HD13	1:A:434:LEU:HD23	1.54	0.90
1:B:379:GLN:OE1	2:D:18:PRO:HG2	1.77	0.83
1:A:391:ILE:CD1	1:A:434:LEU:HD23	2.13	0.78
1:B:417:ALA:HA	1:B:425:ASN:HD21	1.51	0.76
1:A:528:TYR:HA	1:A:533:ILE:HG21	1.69	0.74
1:A:434:LEU:HD11	1:A:502:ARG:HG3	1.74	0.70
1:A:302:PRO:HG2	1:A:305:ILE:HD12	1.75	0.68
1:B:448:PHE:CZ	1:B:452:LYS:HD2	2.28	0.68
1:B:518:TYR:CE2	1:B:522:LEU:HD21	2.30	0.67
1:B:471:GLU:O	1:B:475:GLU:HG3	1.96	0.65
1:B:428:MET:O	1:B:432:GLN:HG3	1.96	0.65
1:B:333:ARG:HB2	1:B:337:GLU:HG3	1.79	0.64
1:A:315:GLU:HB2	1:A:316:PRO:HD3	1.80	0.62
1:A:502:ARG:HD3	1:A:505:GLU:OE1	2.00	0.61
1:A:524:GLY:HA2	1:B:528:TYR:CZ	2.36	0.60
1:B:391:ILE:HD13	1:B:434:LEU:HD23	1.84	0.59
1:A:529:ASN:H	1:A:533:ILE:HD13	1.67	0.59
1:B:391:ILE:CD1	1:B:434:LEU:HD23	2.33	0.59
1:B:357:VAL:HG11	2:D:24:LEU:HD23	1.85	0.58
1:A:533:ILE:HG13	1:A:534:GLU:N	2.18	0.58
1:A:415:ILE:HG23	1:A:419:GLN:NE2	2.18	0.58
1:A:326:LEU:HD11	1:A:348:MET:HB3	1.86	0.58
1:B:323:MET:HE2	1:B:323:MET:O	2.03	0.57
1:A:323:MET:HG2	1:A:407:THR:CB	2.29	0.57
1:B:518:TYR:O	1:B:522:LEU:HD23	2.05	0.57
1:A:326:LEU:HD21	1:A:347:LYS:HB3	1.88	0.56
1:B:384:GLU:OE2	1:B:507:ARG:HG2	2.05	0.56
1:B:417:ALA:HA	1:B:425:ASN:ND2	2.21	0.55
1:B:446:ARG:O	1:B:449:VAL:HG22	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:532:LEU:O	1:B:536:LEU:HD13	2.06	0.54
1:A:315:GLU:O	1:A:319:GLN:HG3	2.07	0.54
1:A:434:LEU:CD1	1:A:502:ARG:HG3	2.37	0.54
1:B:517:LEU:HD23	1:B:536:LEU:HD11	1.90	0.53
1:B:533:ILE:HG22	5:B:197:HOH:O	2.09	0.53
1:A:448:PHE:CZ	1:A:452:LYS:HD2	2.44	0.53
1:A:529:ASN:N	1:A:533:ILE:HD13	2.24	0.52
1:A:347:LYS:HE2	5:B:136:HOH:O	2.09	0.52
1:A:529:ASN:H	1:A:533:ILE:CD1	2.21	0.52
1:B:313:PRO:HG3	5:B:190:HOH:O	2.08	0.52
1:A:437:LYS:O	1:A:441:LEU:HG	2.09	0.52
1:B:364:ILE:HG12	1:B:367:ARG:HH21	1.73	0.52
1:B:467:PHE:O	1:B:471:GLU:HG3	2.10	0.52
1:A:377:LEU:HD23	1:A:461:VAL:HG21	1.91	0.52
5:A:234:HOH:O	2:C:17:ARG:HB2	2.08	0.52
1:B:375:MET:CE	2:D:18:PRO:HD2	2.39	0.52
1:A:330:GLN:HE21	1:A:330:GLN:CA	2.23	0.52
1:A:330:GLN:NE2	1:A:333:ARG:HD2	2.25	0.51
1:A:447:GLU:OE2	1:A:495:LYS:NZ	2.38	0.51
1:B:315:GLU:HB2	1:B:316:PRO:HD3	1.92	0.51
1:B:357:VAL:O	1:B:361:ARG:HG3	2.12	0.50
1:A:333:ARG:HD3	1:A:337:GLU:O	2.11	0.49
1:A:530:ASN:O	1:A:534:GLU:HG3	2.13	0.49
1:B:441:LEU:O	1:B:495:LYS:HE3	2.13	0.49
1:B:375:MET:HE2	2:D:18:PRO:HD2	1.95	0.49
1:A:503:LEU:HB2	1:A:504:PRO:HD3	1.94	0.49
1:A:330:GLN:HE21	1:A:330:GLN:HA	1.78	0.48
1:A:419:GLN:OE1	1:B:335:LYS:HD3	2.14	0.48
1:B:403:ILE:O	1:B:410:GLN:HA	2.13	0.48
1:A:508:ALA:O	1:A:512:GLN:HG3	2.13	0.48
1:B:503:LEU:HB2	1:B:504:PRO:HD3	1.96	0.48
1:A:517:LEU:HG	1:A:536:LEU:HD22	1.95	0.47
1:B:403:ILE:HD11	1:B:413:TYR:OH	2.13	0.47
1:A:353:LEU:HG	1:A:386:LEU:HD11	1.96	0.47
1:A:323:MET:HA	1:A:323:MET:HE2	1.96	0.46
1:B:391:ILE:HD13	1:B:434:LEU:CD2	2.44	0.46
1:B:300:SER:N	5:B:94:HOH:O	2.49	0.46
1:B:420:ALA:CB	1:B:424:LEU:HD23	2.46	0.46
1:A:411:VAL:HG11	1:A:416:ILE:HD11	1.98	0.46
1:A:502:ARG:CD	1:A:505:GLU:OE1	2.63	0.46
1:B:517:LEU:CD2	1:B:536:LEU:HD11	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:GLU:CD	2:D:18:PRO:HB3	2.37	0.44
1:B:312:GLU:HA	1:B:313:PRO:HD3	1.75	0.44
1:B:323:MET:HE2	1:B:327:GLN:HG3	1.99	0.44
1:B:420:ALA:HB1	1:B:424:LEU:HD23	2.00	0.44
1:A:404:PHE:CZ	1:A:408:GLY:HA2	2.53	0.44
1:B:518:TYR:CD2	1:B:522:LEU:HD21	2.52	0.44
1:A:528:TYR:HB2	1:A:533:ILE:HD13	1.98	0.44
1:A:496:PHE:CZ	1:A:500:LEU:HD11	2.53	0.43
1:A:529:ASN:N	1:A:533:ILE:CD1	2.81	0.43
1:B:403:ILE:HD11	1:B:413:TYR:CZ	2.53	0.42
1:B:431:ALA:O	1:B:435:VAL:HG23	2.19	0.42
1:A:364:ILE:HG12	1:A:365:PHE:CD1	2.55	0.42
1:A:341:THR:O	1:A:345:MET:HG2	2.19	0.41
1:B:369:LEU:HD21	1:B:469:LEU:HD22	2.02	0.41
2:C:17:ARG:HA	2:C:18:PRO:HD3	1.92	0.41
2:C:18:PRO:HB2	2:C:21:LEU:HB3	2.02	0.41
1:A:517:LEU:HD23	1:A:536:LEU:HD13	2.02	0.41
1:A:524:GLY:HA2	1:B:528:TYR:CE1	2.56	0.41
1:B:313:PRO:CG	5:B:190:HOH:O	2.66	0.41
1:B:333:ARG:HD3	1:B:337:GLU:O	2.21	0.41
1:B:353:LEU:HG	1:B:386:LEU:HD11	2.03	0.41
1:A:465:GLU:HG3	5:A:228:HOH:O	2.22	0.41
1:A:528:TYR:CZ	1:B:524:GLY:HA2	2.56	0.40
1:A:330:GLN:NE2	1:A:330:GLN:HA	2.36	0.40
1:A:528:TYR:CE1	1:A:529:ASN:ND2	2.89	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	238/255 (93%)	234 (98%)	4 (2%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
2	C	12/14 (86%)	10 (83%)	2 (17%)	0	100	100
2	D	9/14 (64%)	8 (89%)	0	1 (11%)	0	0
All	All	497/538 (92%)	487 (98%)	9 (2%)	1 (0%)	47	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	18	PRO

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	216/229 (94%)	211 (98%)	5 (2%)	50	45
1	B	217/229 (95%)	209 (96%)	8 (4%)	34	25
2	C	11/11 (100%)	11 (100%)	0	100	100
2	D	9/11 (82%)	9 (100%)	0	100	100
All	All	453/480 (94%)	440 (97%)	13 (3%)	42	35

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	323	MET
1	A	330	GLN
1	A	446	ARG
1	A	502	ARG
1	A	532	LEU
1	B	412	ASP
1	B	446	ARG
1	B	469	LEU
1	B	502	ARG
1	B	507	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	522	LEU
1	B	532	LEU
1	B	533	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	GLN
1	A	330	GLN
1	A	432	GLN
1	A	498	GLN
1	B	319	GLN
1	B	327	GLN
1	B	410	GLN
1	B	425	ASN
1	B	430	HIS
1	B	474	GLN
1	B	492	GLN
1	B	512	GLN
1	B	537	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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
4	GOL	A	5001	-	5,5,5	4.54	5 (100%)	5,5,5	5.78	3 (60%)
4	GOL	B	5002	-	5,5,5	4.53	5 (100%)	5,5,5	5.77	3 (60%)
3	EPH	B	1002	-	46,46,48	1.56	8 (17%)	49,51,53	1.36	3 (6%)
4	GOL	B	5003	-	5,5,5	4.55	5 (100%)	5,5,5	5.77	3 (60%)
3	EPH	A	1001	-	46,46,48	1.57	8 (17%)	49,51,53	1.37	3 (6%)

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
4	GOL	A	5001	-	-	2/4/4/4	-
4	GOL	B	5002	-	-	2/4/4/4	-
3	EPH	B	1002	-	-	19/50/50/52	-
4	GOL	B	5003	-	-	3/4/4/4	-
3	EPH	A	1001	-	-	21/50/50/52	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5001	GOL	C3-C2	-7.48	1.21	1.51
4	B	5002	GOL	C3-C2	-7.47	1.21	1.51
4	B	5003	GOL	C3-C2	-7.42	1.21	1.51
4	B	5003	GOL	O1-C1	4.58	1.61	1.42
4	B	5002	GOL	O1-C1	4.56	1.61	1.42
4	A	5001	GOL	O1-C1	4.44	1.61	1.42
3	A	1001	EPH	C25-C24	3.91	1.54	1.31
3	B	1002	EPH	P1-O6	3.90	1.73	1.55
3	A	1001	EPH	P1-O6	3.88	1.73	1.55
3	B	1002	EPH	C25-C24	3.86	1.54	1.31
3	B	1002	EPH	C13-C12	3.77	1.53	1.31
3	A	1001	EPH	C13-C12	3.76	1.53	1.31
3	A	1001	EPH	C29-C28	3.48	1.52	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1002	EPH	C29-C28	3.47	1.51	1.31
3	A	1001	EPH	C16-C15	3.40	1.51	1.31
4	B	5003	GOL	O3-C3	3.39	1.56	1.42
3	B	1002	EPH	C16-C15	3.37	1.51	1.31
4	A	5001	GOL	O3-C3	3.32	1.56	1.42
3	A	1001	EPH	C32-C33	3.27	1.54	1.29
4	B	5002	GOL	O3-C3	3.27	1.56	1.42
3	B	1002	EPH	C32-C33	3.26	1.54	1.29
4	A	5001	GOL	O2-C2	-2.92	1.34	1.43
4	A	5001	GOL	C1-C2	-2.84	1.40	1.51
4	B	5003	GOL	O2-C2	-2.83	1.34	1.43
4	B	5003	GOL	C1-C2	-2.78	1.40	1.51
4	B	5002	GOL	O2-C2	-2.77	1.35	1.43
4	B	5002	GOL	C1-C2	-2.77	1.40	1.51
3	A	1001	EPH	C27-C28	-2.54	1.35	1.50
3	B	1002	EPH	C27-C28	-2.54	1.35	1.50
3	B	1002	EPH	C14-C15	-2.26	1.34	1.51
3	A	1001	EPH	C14-C15	-2.25	1.34	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5001	GOL	O3-C3-C2	10.49	160.49	110.20
4	B	5002	GOL	O3-C3-C2	10.46	160.37	110.20
4	B	5003	GOL	O3-C3-C2	10.45	160.33	110.20
4	A	5001	GOL	O2-C2-C3	6.77	138.93	109.12
4	B	5002	GOL	O2-C2-C3	6.76	138.90	109.12
4	B	5003	GOL	O2-C2-C3	6.75	138.86	109.12
3	A	1001	EPH	C26-C27-C28	5.92	128.45	112.92
3	B	1002	EPH	C26-C27-C28	5.82	128.18	112.92
4	B	5003	GOL	O1-C1-C2	3.29	125.96	110.20
4	B	5002	GOL	O1-C1-C2	3.27	125.87	110.20
4	A	5001	GOL	O1-C1-C2	3.25	125.77	110.20
3	A	1001	EPH	C15-C14-C13	3.23	127.95	112.02
3	B	1002	EPH	C15-C14-C13	3.21	127.84	112.02
3	A	1001	EPH	C31-C32-C33	-2.40	111.99	131.07
3	B	1002	EPH	C31-C32-C33	-2.40	112.01	131.07

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	EPH	C27-C28-C29-C30
3	A	1001	EPH	C9-C10-C11-C12
3	A	1001	EPH	C16-C17-C35-C36
3	B	1002	EPH	C25-C26-C27-C28
3	B	1002	EPH	C27-C28-C29-C30
3	B	1002	EPH	C9-C10-C11-C12
3	B	1002	EPH	C16-C17-C35-C36
4	A	5001	GOL	C1-C2-C3-O3
4	B	5002	GOL	C1-C2-C3-O3
4	B	5003	GOL	C1-C2-C3-O3
3	B	1002	EPH	C4-C18-C19-C20
3	B	1002	EPH	C18-C4-O2-C1
3	A	1001	EPH	C4-C18-C19-C20
3	A	1001	EPH	C18-C4-O2-C1
3	A	1001	EPH	O4-C4-O2-C1
3	B	1002	EPH	O4-C4-O2-C1
4	B	5002	GOL	O1-C1-C2-O2
3	A	1001	EPH	C3-C5-C6-C7
3	B	1002	EPH	C3-C5-C6-C7
3	A	1001	EPH	C14-C15-C16-C17
3	A	1001	EPH	C6-C7-C8-C9
3	B	1002	EPH	C6-C7-C8-C9
3	B	1002	EPH	C7-C8-C9-C10
4	A	5001	GOL	O1-C1-C2-C3
4	B	5003	GOL	O1-C1-C2-C3
3	A	1001	EPH	C7-C8-C9-C10
4	B	5003	GOL	O1-C1-C2-O2
3	A	1001	EPH	C11-C10-C9-C8
3	B	1002	EPH	C11-C10-C9-C8
3	A	1001	EPH	C19-C20-C21-C22
3	B	1002	EPH	C14-C15-C16-C17
3	A	1001	EPH	C20-C21-C22-C23
3	A	1001	EPH	O2-C1-C2-O1
3	A	1001	EPH	C25-C26-C27-C28
3	A	1001	EPH	O2-C1-C2-C37
3	A	1001	EPH	C28-C29-C30-C31
3	A	1001	EPH	C30-C31-C32-C33
3	B	1002	EPH	C28-C29-C30-C31
3	B	1002	EPH	C30-C31-C32-C33
3	B	1002	EPH	C19-C20-C21-C22
3	B	1002	EPH	C20-C21-C22-C23
3	B	1002	EPH	O2-C1-C2-O1
3	A	1001	EPH	C11-C12-C13-C14

Continued on next page...

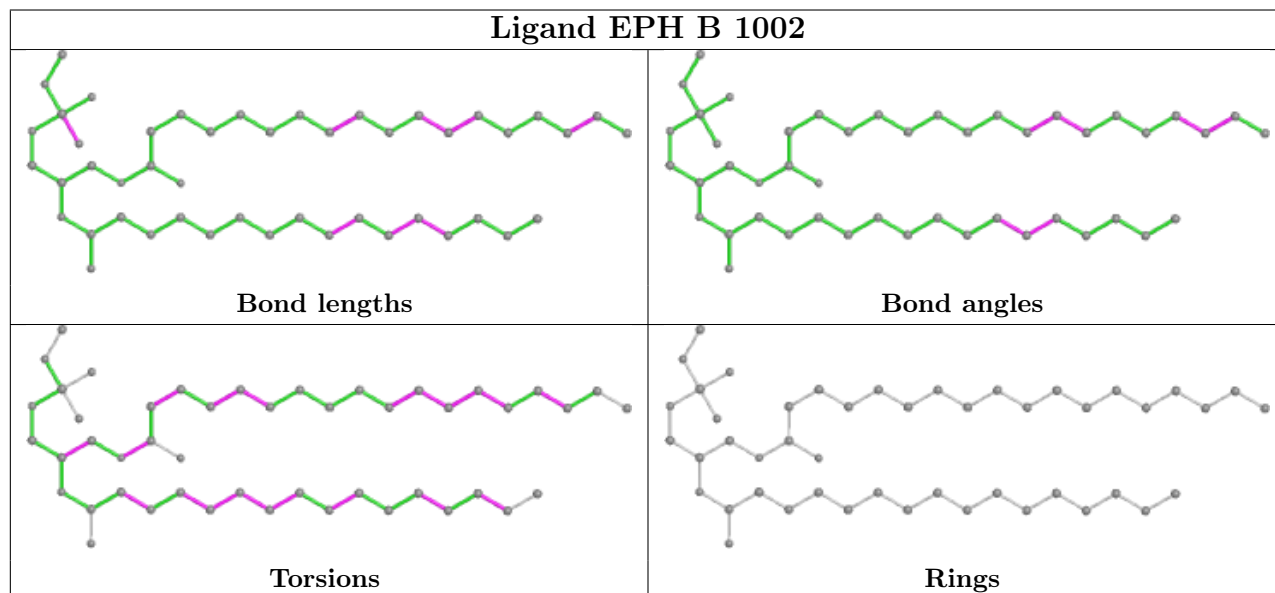
Continued from previous page...

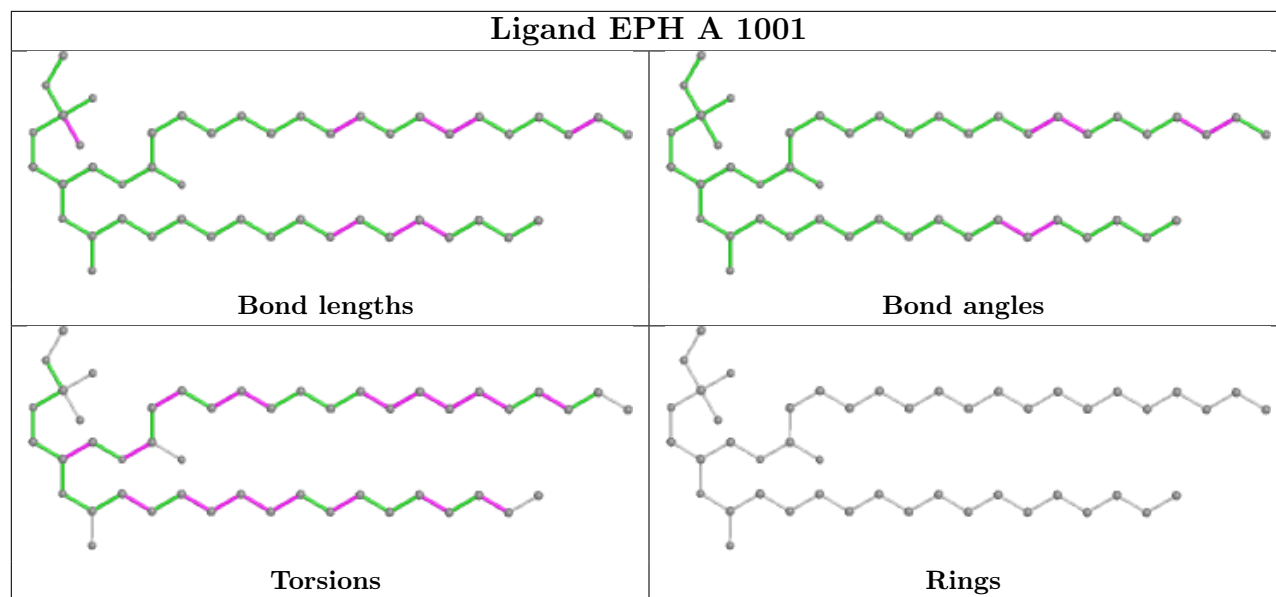
Mol	Chain	Res	Type	Atoms
3	B	1002	EPH	C11-C12-C13-C14
3	A	1001	EPH	C24-C25-C26-C27
3	A	1001	EPH	C26-C27-C28-C29
3	B	1002	EPH	C26-C27-C28-C29

There are no ring outliers.

No monomer is involved in short contacts.

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 [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(Å ²)	Q<0.9
1	A	240/255 (94%)	0.21	10 (4%) 36 39	11, 23, 52, 61	6 (2%)
1	B	240/255 (94%)	0.11	6 (2%) 57 60	14, 23, 43, 52	6 (2%)
2	C	14/14 (100%)	-0.01	2 (14%) 2 2	15, 18, 43, 45	0
2	D	11/14 (78%)	1.01	3 (27%) 0 0	24, 33, 45, 57	0
All	All	505/538 (93%)	0.17	21 (4%) 36 39	11, 23, 46, 61	12 (2%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	519	TYR	5.0
2	D	17	ARG	4.9
1	B	462	LYS	4.0
1	B	300	SER	3.9
1	A	418	SER	3.2
1	A	415	ILE	3.0
1	A	414	SER	3.0
1	B	413	TYR	2.9
1	B	419	GLN	2.7
1	B	467	PHE	2.7
2	D	22	TYR	2.6
2	C	15	ALA	2.5
2	D	18	PRO	2.5
1	A	299	ALA	2.3
1	B	430	HIS	2.3
1	A	419	GLN	2.3
1	A	413	TYR	2.2
1	A	462	LYS	2.2
1	A	518	TYR	2.0
2	C	16	SER	2.0
1	A	537	HIS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.