Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 03:11 PM BST

PDB ID	:	5HJP
Title	:	Identification of LXRbeta selective agonists for the treatment of Alzheimer's Disease
Authors	:	Parthasarathy, G.; Klein, D.
Deposited on	:	2016-01-13
Resolution	:	2.60 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 following versions of software and data (see references ⓘ) were used in the production of this report:

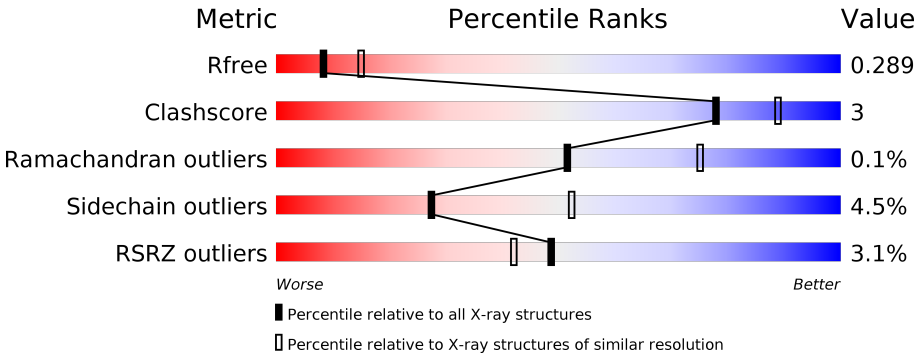
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	254	6% 74% 10% 15%
1	C	254	4% 78% 6% 15%
2	B	264	81% 16%
2	D	264	2% 87% 8% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7679 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 Retinoic acid receptor RXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1715	1101	300	304	10			
1	C	216	Total	C	N	O	S	0	0	0
			1722	1106	301	305	10			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	GLY	-	expression tag	UNP P28702
A	535	SER	-	expression tag	UNP P28702
A	536	GLY	-	expression tag	UNP P28702
A	537	SER	-	expression tag	UNP P28702
A	538	GLY	-	expression tag	UNP P28702
A	539	SER	-	expression tag	UNP P28702
A	540	HIS	-	expression tag	UNP P28702
A	541	LYS	-	expression tag	UNP P28702
A	542	ILE	-	expression tag	UNP P28702
A	543	LEU	-	expression tag	UNP P28702
A	544	HIS	-	expression tag	UNP P28702
A	545	ARG	-	expression tag	UNP P28702
A	546	LEU	-	expression tag	UNP P28702
A	547	LEU	-	expression tag	UNP P28702
A	548	GLN	-	expression tag	UNP P28702
A	549	ASP	-	expression tag	UNP P28702
A	550	SER	-	expression tag	UNP P28702
A	551	SER	-	expression tag	UNP P28702
A	552	SER	-	expression tag	UNP P28702
C	534	GLY	-	expression tag	UNP P28702
C	535	SER	-	expression tag	UNP P28702
C	536	GLY	-	expression tag	UNP P28702
C	537	SER	-	expression tag	UNP P28702
C	538	GLY	-	expression tag	UNP P28702
C	539	SER	-	expression tag	UNP P28702

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Chain	Residue	Modelled	Actual	Comment	Reference
C	540	HIS	-	expression tag	UNP P28702
C	541	LYS	-	expression tag	UNP P28702
C	542	ILE	-	expression tag	UNP P28702
C	543	LEU	-	expression tag	UNP P28702
C	544	HIS	-	expression tag	UNP P28702
C	545	ARG	-	expression tag	UNP P28702
C	546	LEU	-	expression tag	UNP P28702
C	547	LEU	-	expression tag	UNP P28702
C	548	GLN	-	expression tag	UNP P28702
C	549	ASP	-	expression tag	UNP P28702
C	550	SER	-	expression tag	UNP P28702
C	551	SER	-	expression tag	UNP P28702
C	552	SER	-	expression tag	UNP P28702

- Molecule 2 is a protein called Oxysterols receptor LXR-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	259	Total	C	N	O	S	0	0	0
			2079	1323	367	382	7			
2	D	251	Total	C	N	O	S	0	0	0
			2033	1296	359	371	7			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	259	ALA	GLN	engineered mutation	UNP P55055
B	261	GLY	ARG	engineered mutation	UNP P55055
B	262	SER	ASP	engineered mutation	UNP P55055
B	264	SER	ARG	engineered mutation	UNP P55055
B	462	GLY	-	expression tag	UNP P55055
B	463	SER	-	expression tag	UNP P55055
B	464	GLY	-	expression tag	UNP P55055
B	465	SER	-	expression tag	UNP P55055
B	466	GLY	-	expression tag	UNP P55055
B	467	SER	-	expression tag	UNP P55055
B	468	HIS	-	expression tag	UNP P55055
B	469	LYS	-	expression tag	UNP P55055
B	470	ILE	-	expression tag	UNP P55055
B	471	LEU	-	expression tag	UNP P55055
B	472	HIS	-	expression tag	UNP P55055
B	473	ARG	-	expression tag	UNP P55055
B	474	LEU	-	expression tag	UNP P55055

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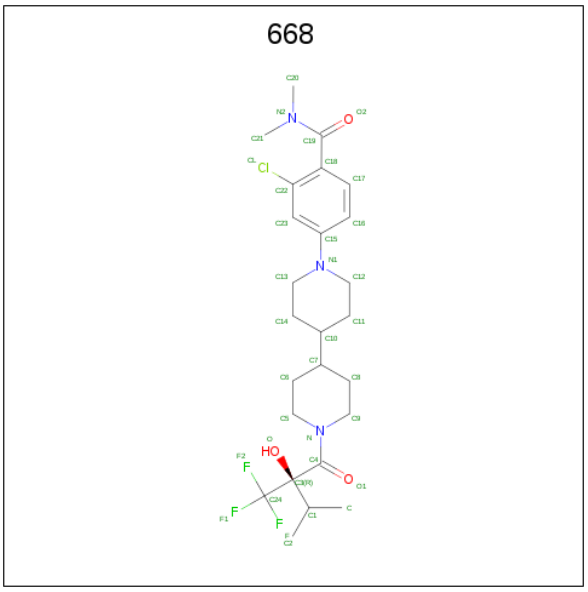
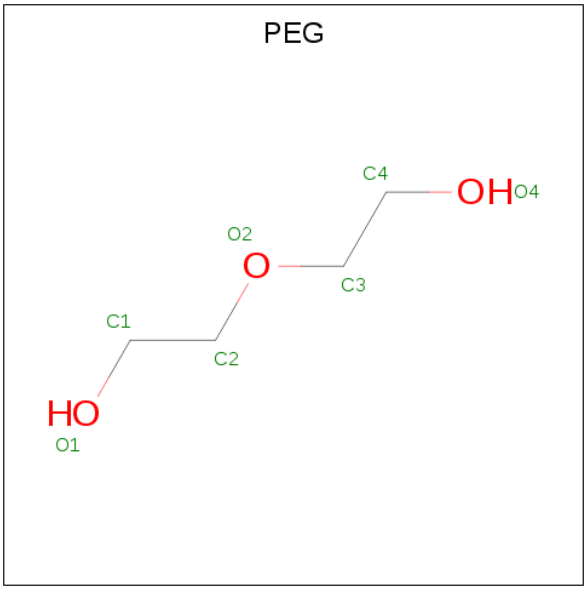
Chain	Residue	Modelled	Actual	Comment	Reference
B	475	LEU	-	expression tag	UNP P55055
B	476	GLN	-	expression tag	UNP P55055
B	477	ASP	-	expression tag	UNP P55055
B	478	SER	-	expression tag	UNP P55055
B	479	SER	-	expression tag	UNP P55055
B	480	SER	-	expression tag	UNP P55055
D	259	ALA	GLN	engineered mutation	UNP P55055
D	261	GLY	ARG	engineered mutation	UNP P55055
D	262	SER	ASP	engineered mutation	UNP P55055
D	264	SER	ARG	engineered mutation	UNP P55055
D	462	GLY	-	expression tag	UNP P55055
D	463	SER	-	expression tag	UNP P55055
D	464	GLY	-	expression tag	UNP P55055
D	465	SER	-	expression tag	UNP P55055
D	466	GLY	-	expression tag	UNP P55055
D	467	SER	-	expression tag	UNP P55055
D	468	HIS	-	expression tag	UNP P55055
D	469	LYS	-	expression tag	UNP P55055
D	470	ILE	-	expression tag	UNP P55055
D	471	LEU	-	expression tag	UNP P55055
D	472	HIS	-	expression tag	UNP P55055
D	473	ARG	-	expression tag	UNP P55055
D	474	LEU	-	expression tag	UNP P55055
D	475	LEU	-	expression tag	UNP P55055
D	476	GLN	-	expression tag	UNP P55055
D	477	ASP	-	expression tag	UNP P55055
D	478	SER	-	expression tag	UNP P55055
D	479	SER	-	expression tag	UNP P55055
D	480	SER	-	expression tag	UNP P55055

- Molecule 3 is 2-chloro-4-{1'-[(2R)-2-hydroxy-3-methyl-2-(trifluoromethyl)butanoyl]-4,4'-bipiperidin-1-yl}-N,N-dimethylbenzamide (three-letter code: 668) (formula: $C_{25}H_{35}ClF_3N_3O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	F	N	O	0	0
			35	25	1	3	3	3		
3	D	1	Total	C	Cl	F	N	O	0	0
			35	25	1	3	3	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

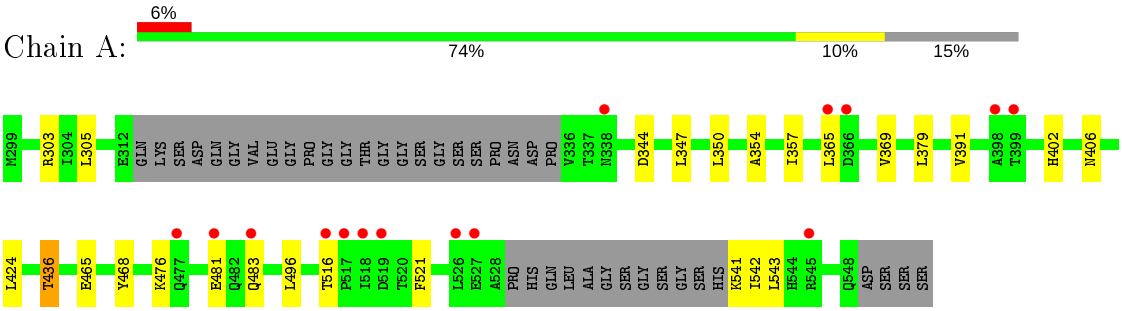
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	15	Total O 15 15	0	0
5	C	11	Total O 11 11	0	0
5	D	16	Total O 16 16	0	0

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.

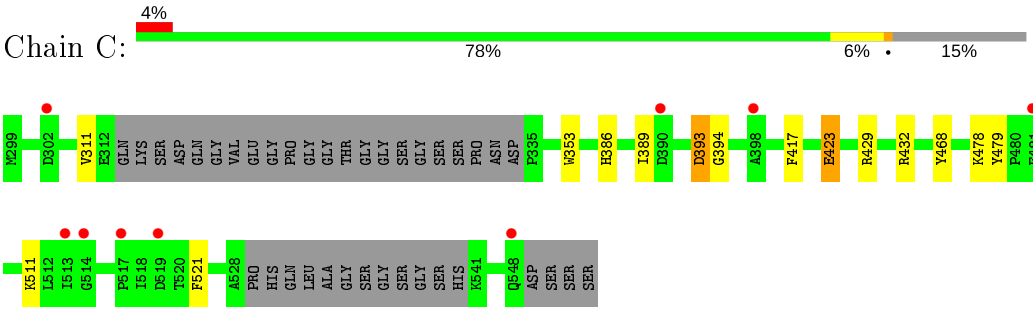
- Molecule 1: Retinoic acid receptor RXR-beta

Chain A:



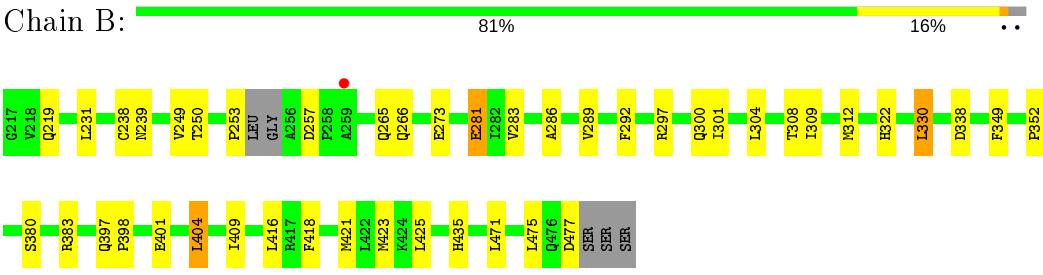
- Molecule 1: Retinoic acid receptor RXR-beta

Chain C:



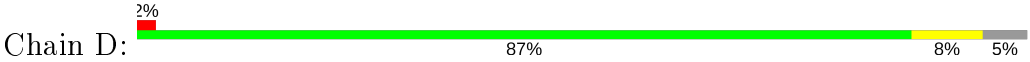
- Molecule 2: Oxysterols receptor LXR-beta

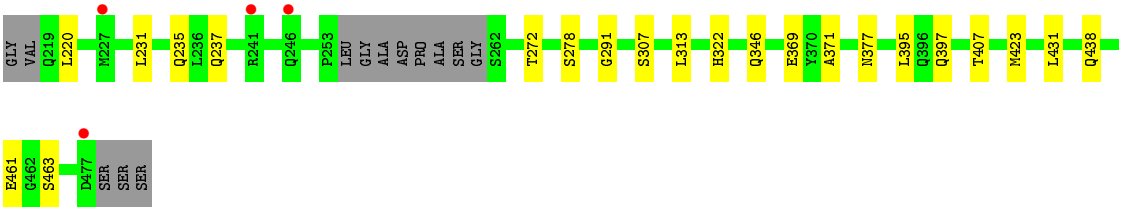
Chain B:



- Molecule 2: Oxysterols receptor LXR-beta

Chain D:




GLY
VAL
Q219
L220
M227
L231
Q235
L236
Q237
R241
Q246
P253
LEU
GLY
ALA
ASP
PRO
ALA
SER
GLY
S262
T272
S278
G291
S307
L313
H322
Q346
E369
Y370
A371
N377
L395
Q396
Q397
T407
M423
L431
Q438
E461
G462
S463
D477
SER
SER
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	66.77Å 106.03Å 139.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.70 – 2.60 35.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (35.70-2.60) 96.4 (35.70-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.61Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.5	Depositor
R, R_{free}	0.236 , 0.283 0.236 , 0.289	Depositor DCC
R_{free} test set	1525 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7679	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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, 0.333 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: PEG, 668

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	0.45	0/1744	0.64	0/2351
1	C	0.49	0/1752	0.66	0/2362
2	B	0.49	0/2120	0.68	0/2866
2	D	0.49	0/2073	0.65	0/2801
All	All	0.48	0/7689	0.66	0/10380

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

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	1715	0	1775	11	0
1	C	1722	0	1783	8	0
2	B	2079	0	2095	21	0
2	D	2033	0	2054	7	0
3	B	35	0	0	1	0
3	D	35	0	0	0	0
4	B	7	0	10	0	0
4	C	7	0	10	0	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	15	0	0	0	0
5	C	11	0	0	0	0
5	D	16	0	0	0	0
All	All	7679	0	7727	44	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 3.

All (44) 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:476:LYS:HE2	1:A:483:GLN:HE22	1.57	0.69
1:C:423:GLU:HG3	1:C:492:ARG:HH12	1.59	0.67
2:B:250:THR:HG23	2:B:273:GLU:OE1	1.95	0.66
2:B:292:PHE:CZ	2:B:300:GLN:HB2	2.33	0.63
1:A:468:TYR:OH	2:B:423:MET:HG3	2.00	0.61
1:A:424:LEU:HD21	1:A:496:LEU:HD13	1.84	0.60
1:C:468:TYR:OH	2:D:423:MET:HG3	2.08	0.54
2:D:307:SER:HB2	2:D:377:ASN:OD1	2.07	0.54
2:B:286:ALA:HA	2:B:289:VAL:HG12	1.90	0.54
2:B:301:ILE:HG23	2:B:471:LEU:HD23	1.90	0.53
2:D:313:LEU:HD13	2:D:431:LEU:HD23	1.92	0.52
1:A:354:ALA:O	1:A:357:ILE:HG13	2.11	0.51
1:C:311:VAL:HG11	1:C:353:TRP:HB2	1.93	0.50
1:C:423:GLU:HG3	1:C:492:ARG:NH1	2.27	0.50
2:B:309:ILE:HG12	2:B:435:HIS:CG	2.47	0.49
2:B:238:CYS:HB3	2:B:281:GLU:HG2	1.95	0.48
1:C:389:ILE:O	1:C:429:ARG:HD3	2.14	0.48
2:B:304:LEU:HD12	2:B:475:LEU:HD21	1.96	0.48
1:A:350:LEU:HD11	1:A:379:LEU:HD13	1.97	0.47
2:B:283:VAL:HG12	2:B:304:LEU:HD13	1.97	0.47
2:D:369:GLU:OE1	2:D:407:THR:HG22	2.15	0.47
1:C:478:LYS:HG2	1:C:479:TYR:CE2	2.50	0.46
1:A:344:ASP:HA	1:A:347:LEU:HD12	1.97	0.46
1:A:305:LEU:HB2	1:A:436:THR:HG23	1.98	0.46
1:A:541:LYS:HD2	1:A:542:ILE:HG13	1.98	0.46
2:B:253:PRO:HG3	2:B:266:GLN:HB3	1.98	0.46
2:B:308:THR:O	2:B:312:MET:HG3	2.17	0.45
2:B:404:LEU:HD23	2:B:418:PHE:CD2	2.52	0.45
2:B:330:LEU:HD13	3:B:501:668:CL	2.54	0.44
2:B:239:ASN:OD1	2:B:281:GLU:OE1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:GLY:HA3	2:D:395:LEU:HD22	2.00	0.44
2:B:297:ARG:HA	2:B:300:GLN:HG2	2.00	0.43
2:D:231:LEU:HB3	2:D:371:ALA:HB1	2.01	0.43
2:D:346:GLN:HG2	2:D:438:GLN:OE1	2.18	0.43
2:B:398:PRO:HA	2:B:401:GLU:HG2	2.00	0.43
2:B:380:SER:O	2:B:383:ARG:HG2	2.18	0.43
1:A:369:VAL:HG13	1:A:543:LEU:HD23	2.01	0.42
2:B:231:LEU:HB3	2:B:371:ALA:HB1	2.01	0.42
2:B:377:ASN:HD22	2:B:425:LEU:HD22	1.85	0.41
1:C:386:HIS:O	1:C:389:ILE:HG12	2.21	0.41
1:A:465:GLU:HA	1:A:468:TYR:CD2	2.56	0.41
2:B:349:PHE:C	2:B:352:PRO:HD2	2.41	0.41
1:C:394:GLY:HA2	1:C:417:PHE:HZ	1.86	0.41
1:A:465:GLU:HB3	2:B:416:LEU:HD13	2.03	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	209/254 (82%)	204 (98%)	5 (2%)	0	100 100
1	C	210/254 (83%)	202 (96%)	7 (3%)	1 (0%)	29 52
2	B	255/264 (97%)	246 (96%)	9 (4%)	0	100 100
2	D	247/264 (94%)	243 (98%)	4 (2%)	0	100 100
All	All	921/1036 (89%)	895 (97%)	25 (3%)	1 (0%)	51 75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	393	ASP

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	188/216 (87%)	179 (95%)	9 (5%)	25	49
1	C	189/216 (88%)	183 (97%)	6 (3%)	39	65
2	B	227/231 (98%)	214 (94%)	13 (6%)	20	41
2	D	223/231 (96%)	214 (96%)	9 (4%)	31	57
All	All	827/894 (92%)	790 (96%)	37 (4%)	27	52

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	ARG
1	A	365	LEU
1	A	391	VAL
1	A	402	HIS
1	A	406	ASN
1	A	436	THR
1	A	481	GLU
1	A	516	THR
1	A	521	PHE
2	B	219	GLN
2	B	249	VAL
2	B	257	ASP
2	B	265	GLN
2	B	281	GLU
2	B	322	HIS
2	B	330	LEU
2	B	338	ASP
2	B	397	GLN
2	B	404	LEU
2	B	409	ILE
2	B	421	MET
2	B	477	ASP
1	C	393	ASP
1	C	423	GLU

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Mol	Chain	Res	Type
1	C	432	ARG
1	C	498	SER
1	C	511	LYS
1	C	521	PHE
2	D	220	LEU
2	D	235	GLN
2	D	237	GLN
2	D	272	THR
2	D	278	SER
2	D	322	HIS
2	D	397	GLN
2	D	461	GLU
2	D	463	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	483	GLN
2	B	239	ASN
2	B	265	GLN
2	B	377	ASN
2	B	397	GLN

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

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	668	B	501	-	36,37,37	1.10	3 (8%)	48,56,56	1.25	4 (8%)
4	PEG	B	502	-	6,6,6	0.27	0	5,5,5	0.27	0
3	668	D	501	-	36,37,37	1.05	4 (11%)	48,56,56	1.09	4 (8%)
4	PEG	C	601	-	6,6,6	0.30	0	5,5,5	0.24	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	668	B	501	-	-	4/40/61/61	0/3/3/3
4	PEG	B	502	-	-	1/4/4/4	-
3	668	D	501	-	-	14/40/61/61	0/3/3/3
4	PEG	C	601	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	668	C13-N1	3.87	1.52	1.46
3	B	501	668	C12-N1	3.63	1.52	1.46
3	B	501	668	C15-N1	3.51	1.48	1.38
3	D	501	668	C15-N1	3.51	1.48	1.38
3	D	501	668	C13-N1	3.25	1.51	1.46
3	D	501	668	C12-N1	3.12	1.51	1.46
3	D	501	668	C10-C7	2.15	1.61	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	668	C12-N1-C13	5.84	124.41	111.52
3	D	501	668	O1-C4-C3	-3.21	110.45	118.69
3	B	501	668	O1-C4-C3	-2.93	111.17	118.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	501	668	C24-C3-C4	-2.67	103.99	108.47
3	B	501	668	C9-C8-C7	2.40	114.34	109.29
3	D	501	668	C5-N-C4	2.31	133.80	123.69
3	B	501	668	C23-C15-N1	-2.28	118.88	121.33
3	D	501	668	C23-C15-N1	-2.27	118.90	121.33

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	668	C24-C3-C4-O1
3	B	501	668	C24-C3-C4-N
3	D	501	668	F2-C24-C3-O
3	D	501	668	F2-C24-C3-C1
3	D	501	668	F2-C24-C3-C4
3	D	501	668	F-C24-C3-O
3	D	501	668	F-C24-C3-C1
3	D	501	668	F-C24-C3-C4
3	D	501	668	F1-C24-C3-O
3	D	501	668	F1-C24-C3-C1
3	D	501	668	F1-C24-C3-C4
3	B	501	668	C14-C10-C7-C6
4	B	502	PEG	C4-C3-O2-C2
3	D	501	668	C24-C3-C4-O1
4	C	601	PEG	C4-C3-O2-C2
3	D	501	668	C24-C3-C4-N
4	C	601	PEG	C1-C2-O2-C3
3	D	501	668	C14-C10-C7-C6
3	B	501	668	O-C3-C4-O1
3	D	501	668	O-C3-C4-O1
3	D	501	668	C16-C15-N1-C12

There are no ring outliers.

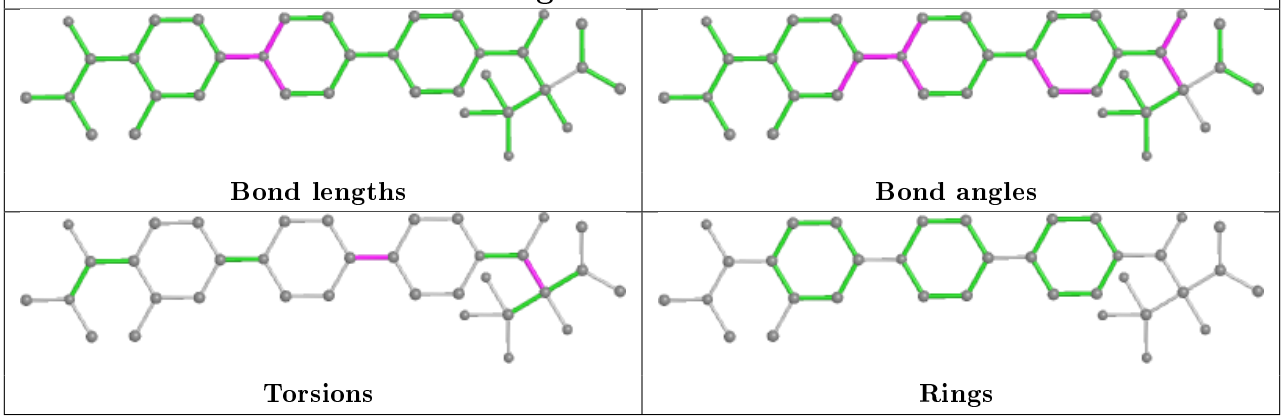
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	668	1	0

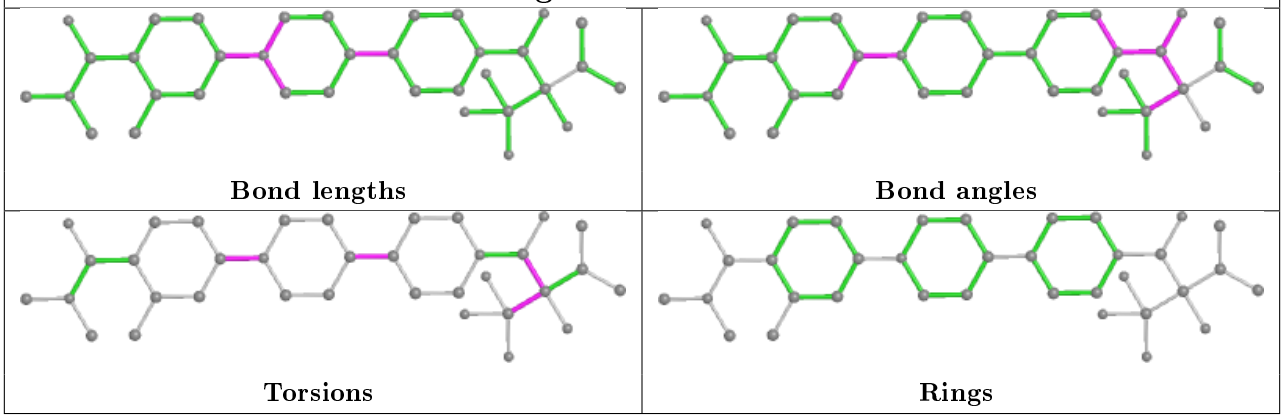
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less 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 668 B 501



Ligand 668 D 501



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	215/254 (84%)	0.53	15 (6%)	16 12	35, 61, 86, 92	0
1	C	216/254 (85%)	0.20	9 (4%)	36 29	25, 44, 65, 90	0
2	B	259/264 (98%)	-0.03	1 (0%)	92 91	27, 39, 56, 68	0
2	D	251/264 (95%)	-0.03	4 (1%)	72 68	22, 37, 55, 72	0
All	All	941/1036 (90%)	0.15	29 (3%)	49 42	22, 42, 72, 92	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	514	GLY	7.8
1	A	399	THR	4.3
2	D	477	ASP	4.1
1	C	390	ASP	3.7
1	A	477	GLN	3.7
1	C	519	ASP	3.6
1	A	398	ALA	3.5
1	C	517	PRO	3.3
1	C	481	GLU	3.1
1	C	398	ALA	3.1
1	A	545	ARG	2.9
1	A	518	ILE	2.9
1	A	517	PRO	2.9
1	C	513	ILE	2.8
1	A	527	GLU	2.7
1	C	302	ASP	2.6
1	A	365	LEU	2.5
1	A	483	GLN	2.5
2	D	246	GLN	2.4
1	A	481	GLU	2.2
2	D	227	MET	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	241	ARG	2.2
2	B	259	ALA	2.2
1	C	548	GLN	2.1
1	A	519	ASP	2.1
1	A	516	THR	2.1
1	A	338	ASN	2.0
1	A	366	ASP	2.0
1	A	526	LEU	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)

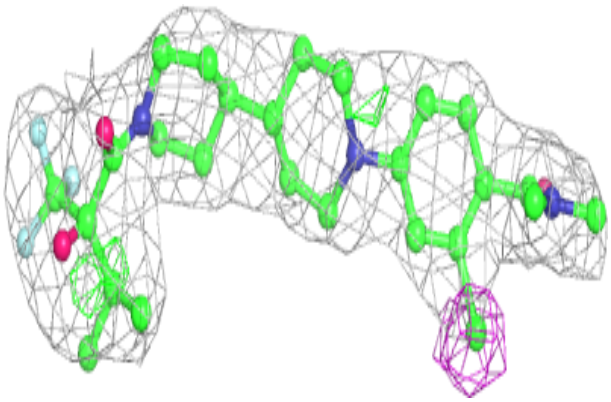
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

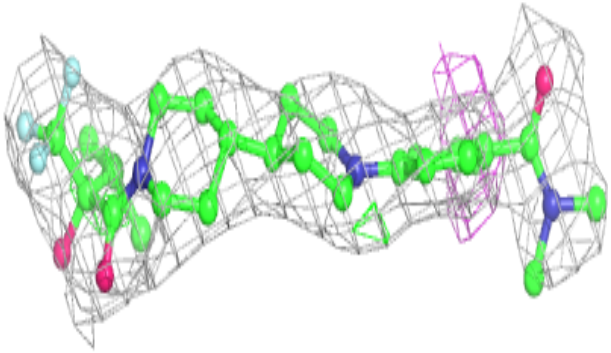
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	668	B	501	35/35	0.82	0.24	38,47,60,63	0
4	PEG	B	502	7/7	0.84	0.17	49,53,55,55	0
3	668	D	501	35/35	0.90	0.18	26,42,54,62	0
4	PEG	C	601	7/7	0.91	0.16	37,39,43,45	0

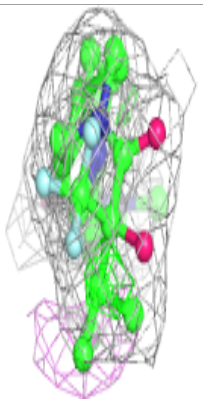
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 668 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)

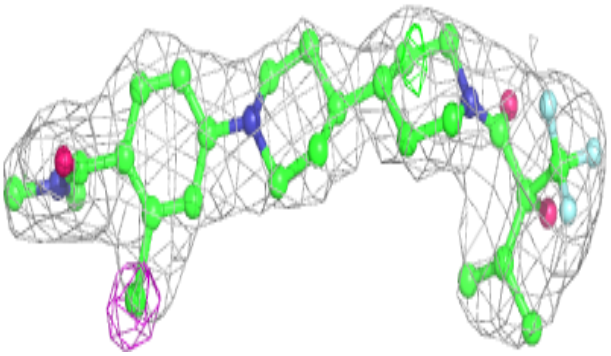


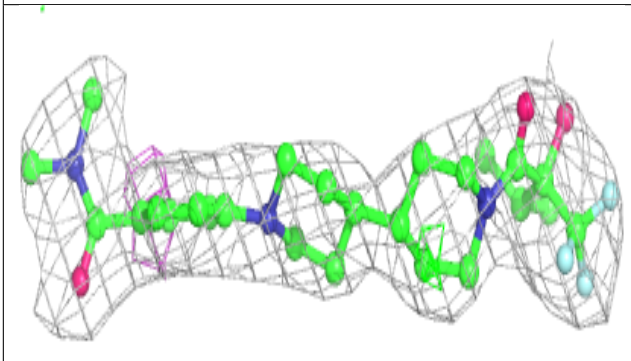


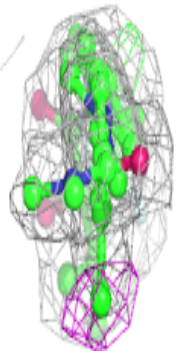


Electron density around 668 D 501:

$2mF_o$-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.