



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:44 PM UTC

PDB ID : 2Q6B / pdb_00002q6b
Title : Design and synthesis of novel, conformationally restricted HMG-COA reductase inhibitors
Authors : Pavlovsky, A.; Pfefferkorn, J.A.; Harris, M.S.; Finzel, B.C.
Deposited on : 2007-06-04
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

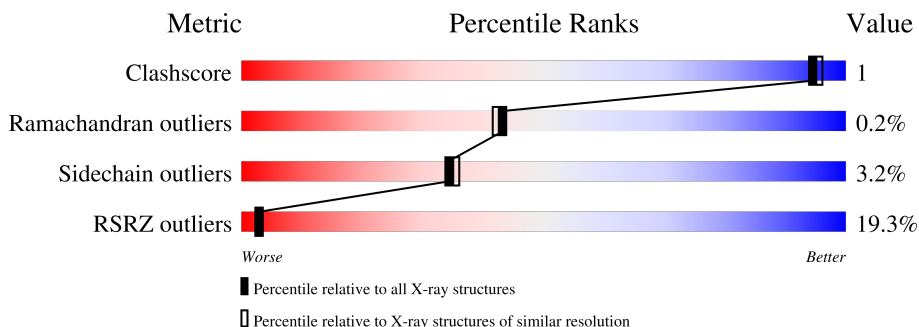
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	441	21% 89% 7% .
1	B	441	19% 90% 5% .
1	C	441	15% 91% . .
1	D	441	19% 91% 5% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13820 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 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3167	1974	558	605	30			
1	B	423	Total	C	N	O	S	0	0	0
			3148	1962	553	603	30			
1	C	422	Total	C	N	O	S	0	0	0
			3139	1957	552	600	30			
1	D	418	Total	C	N	O	S	0	0	0
			3113	1940	549	594	30			

There are 28 discrepancies between the modelled and reference sequences:

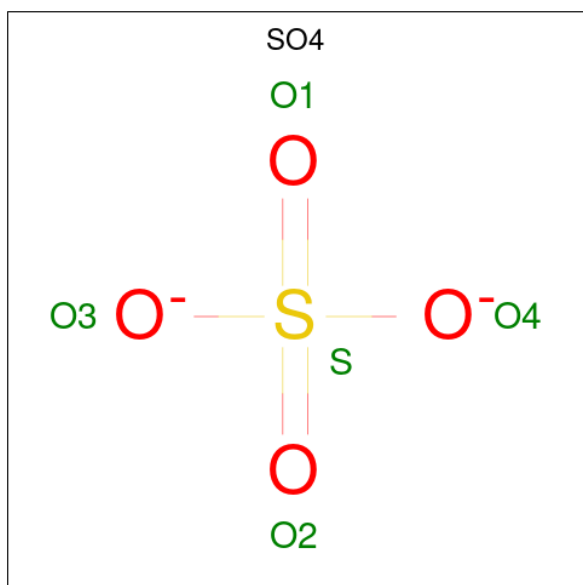
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	435	HIS	-	expression tag	UNP P04035
B	436	HIS	-	expression tag	UNP P04035
B	437	HIS	-	expression tag	UNP P04035
B	438	HIS	-	expression tag	UNP P04035
B	439	HIS	-	expression tag	UNP P04035
B	440	HIS	-	expression tag	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	435	HIS	-	expression tag	UNP P04035
C	436	HIS	-	expression tag	UNP P04035
C	437	HIS	-	expression tag	UNP P04035
C	438	HIS	-	expression tag	UNP P04035
C	439	HIS	-	expression tag	UNP P04035
C	440	HIS	-	expression tag	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035

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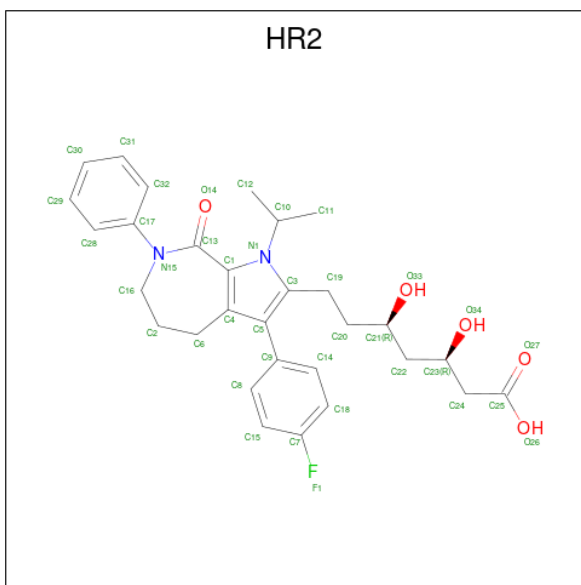
Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is (3R,5R)-7-[3-(4-FLUOROPHENYL)-1-ISOPROPYL-8-OXO-7-PHENYL-1,4,5,6,7,8-HEXAHYDROPYRROLO[2,3-C]AZEPIN-2-YL]-3,5-DIHYDROXYHEPTANOIC ACID (CCD ID: HR2) (formula: C₃₀H₃₅N₂O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 38	C 30	F 1	N 2	O 5	0	0
3	A	1	Total 38	C 30	F 1	N 2	O 5	0	0
3	C	1	Total 38	C 30	F 1	N 2	O 5	0	0
3	D	1	Total 38	C 30	F 1	N 2	O 5	0	0

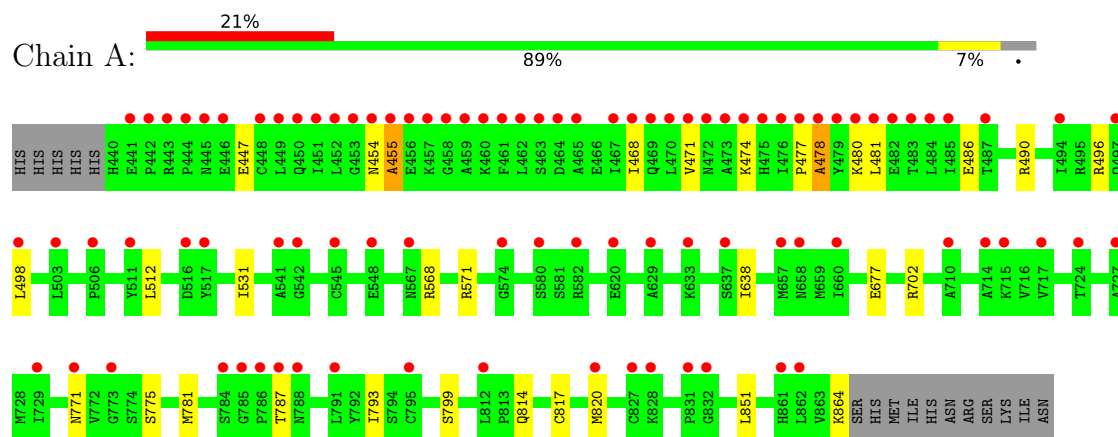
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	260	Total O 260 260	0	0
4	B	251	Total O 251 251	0	0
4	C	285	Total O 285 285	0	0
4	D	285	Total O 285 285	0	0

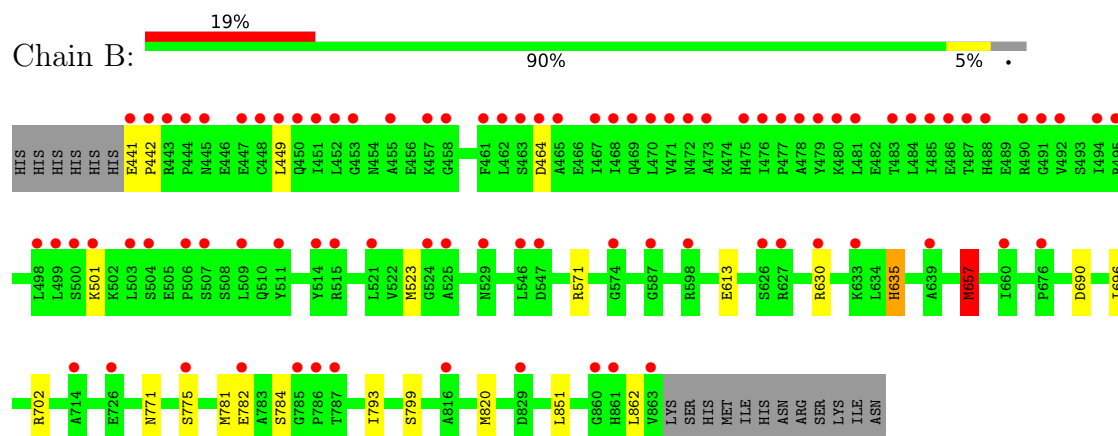
3 Residue-property plots [i](#)

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.

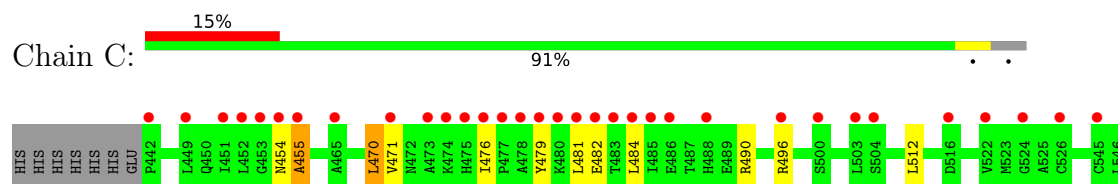
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

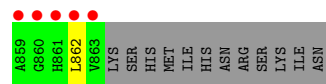


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase

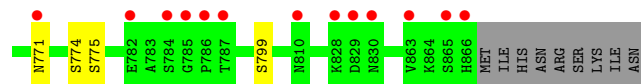


- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase





Chain D: 19% 91% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.72Å 133.19Å 82.67Å 90.00° 92.63° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.00) 91.4 (30.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.256 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for l,k,-h 0.037 for h,-k,-l 0.033 for l,-k,h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13820	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: HR2, SO4

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	0.43	0/3214	0.77	0/4345
1	B	0.43	1/3194 (0.0%)	0.75	0/4319
1	C	0.42	0/3185	0.77	0/4306
1	D	0.43	0/3159	0.76	0/4269
All	All	0.43	1/12752 (0.0%)	0.76	0/17239

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	657	MET	SD-CE	-5.89	1.64	1.79

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	3167	0	3207	11	0
1	B	3148	0	3187	10	0
1	C	3139	0	3182	9	0
1	D	3113	0	3151	3	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	76	0	68	0	0
3	C	38	0	34	1	0
3	D	38	0	34	1	0
4	A	260	0	0	0	0
4	B	251	0	0	0	0
4	C	285	0	0	0	0
4	D	285	0	0	0	0
All	All	13820	0	12863	33	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 1.

All (33) 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:C:471:VAL:HG21	1:C:481:LEU:HD11	1.73	0.70
1:C:771:ASN:OD1	1:C:775:SER:OG	2.12	0.67
1:A:771:ASN:OD1	1:A:775:SER:OG	2.22	0.57
1:C:470:LEU:HB3	1:C:476:ILE:HG21	1.91	0.52
1:A:477:PRO:O	1:A:478:ALA:HB2	2.10	0.51
1:B:771:ASN:OD1	1:B:775:SER:OG	2.29	0.51
1:B:781:MET:HE2	1:B:793:ILE:HD12	1.93	0.51
1:D:771:ASN:OD1	1:D:775:SER:OG	2.28	0.51
1:A:454:ASN:O	1:A:455:ALA:HB3	2.11	0.50
1:B:635:HIS:CD2	1:B:635:HIS:C	2.89	0.50
1:C:471:VAL:CG2	1:C:481:LEU:HD11	2.42	0.50
1:A:781:MET:HE2	1:A:793:ILE:HD12	1.94	0.50
1:C:454:ASN:O	1:C:455:ALA:HB3	2.11	0.50
1:C:476:ILE:HD11	1:C:484:LEU:HD22	1.94	0.48
1:C:496:ARG:NH1	1:C:512:LEU:O	2.47	0.48
1:B:657:MET:HE2	1:B:690:ASP:CG	2.38	0.47
1:B:441:GLU:N	1:B:442:PRO:CD	2.79	0.45
3:C:3003:HR2:O14	3:C:3003:HR2:H113	2.16	0.45
1:A:817:CYS:HA	1:A:820:MET:HE3	1.99	0.45
3:D:3004:HR2:O14	3:D:3004:HR2:H113	2.16	0.44
1:C:454:ASN:O	1:C:455:ALA:CB	2.64	0.44
1:B:782:GLU:OE2	1:C:641:ARG:HD3	2.18	0.44
1:D:560:GLY:O	1:D:561:CYS:HB2	2.18	0.44
1:A:477:PRO:O	1:A:478:ALA:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ILE:HD11	1:B:820:MET:HE1	2.00	0.43
1:B:793:ILE:HD13	1:B:851:LEU:HG	2.00	0.43
1:D:774:SER:HA	1:D:799:SER:O	2.19	0.43
1:A:454:ASN:O	1:A:455:ALA:CB	2.67	0.43
1:A:702:ARG:O	1:A:799:SER:HA	2.19	0.43
1:A:793:ILE:HD13	1:A:851:LEU:HG	2.00	0.43
1:B:702:ARG:O	1:B:799:SER:HA	2.19	0.42
1:B:635:HIS:CE1	1:B:696:ILE:HD11	2.55	0.41
1:A:471:VAL:HG21	1:A:481:LEU:HD11	2.02	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	423/441 (96%)	402 (95%)	19 (4%)	2 (0%)	24	21
1	B	421/441 (96%)	404 (96%)	17 (4%)	0	100	100
1	C	420/441 (95%)	403 (96%)	15 (4%)	2 (0%)	24	21
1	D	414/441 (94%)	401 (97%)	13 (3%)	0	100	100
All	All	1678/1764 (95%)	1610 (96%)	64 (4%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	478	ALA
1	A	455	ALA
1	C	455	ALA
1	C	479	TYR

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	339/355 (96%)	323 (95%)	16 (5%)	23	22
1	B	337/355 (95%)	326 (97%)	11 (3%)	33	34
1	C	336/355 (95%)	329 (98%)	7 (2%)	47	52
1	D	334/355 (94%)	325 (97%)	9 (3%)	39	42
All	All	1346/1420 (95%)	1303 (97%)	43 (3%)	34	35

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	GLU
1	A	468	ILE
1	A	474	LYS
1	A	480	LYS
1	A	486	GLU
1	A	490	ARG
1	A	496	ARG
1	A	498	LEU
1	A	512	LEU
1	A	568	ARG
1	A	571	ARG
1	A	638	ILE
1	A	677	GLU
1	A	787	THR
1	A	814	GLN
1	A	864	LYS
1	B	449	LEU
1	B	464	ASP
1	B	501	LYS
1	B	523	MET
1	B	571	ARG
1	B	613	GLU
1	B	630	ARG
1	B	635	HIS

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Mol	Chain	Res	Type
1	B	657	MET
1	B	784	SER
1	B	862	LEU
1	C	470	LEU
1	C	482	GLU
1	C	490	ARG
1	C	571	ARG
1	C	627	ARG
1	C	802	ILE
1	C	862	LEU
1	D	466	GLU
1	D	470	LEU
1	D	475	HIS
1	D	482	GLU
1	D	484	LEU
1	D	487	THR
1	D	613	GLU
1	D	638	ILE
1	D	677	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	445	ASN
1	A	472	ASN
1	A	475	HIS
1	A	510	GLN
1	A	518	ASN
1	A	567	ASN
1	A	736	ASN
1	A	861	HIS
1	B	445	ASN
1	B	472	ASN
1	B	510	GLN
1	B	632	GLN
1	B	736	ASN
1	B	861	HIS
1	C	472	ASN
1	C	475	HIS
1	C	488	HIS
1	C	497	GLN
1	C	632	GLN

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Mol	Chain	Res	Type
1	D	445	ASN
1	D	450	GLN
1	D	472	ASN
1	D	475	HIS
1	D	632	GLN
1	D	819	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	$\# Z > 2$
2	SO4	D	2004	-	4,4,4	0.23	0	6,6,6	0.18	0
3	HR2	C	3003	-	40,41,41	1.22	5 (12%)	42,58,58	1.32	4 (9%)
3	HR2	A	3002	-	40,41,41	1.20	5 (12%)	42,58,58	1.30	3 (7%)
2	SO4	A	2001	-	4,4,4	0.22	0	6,6,6	0.14	0
3	HR2	A	3001	-	40,41,41	1.20	5 (12%)	42,58,58	1.29	3 (7%)
2	SO4	B	2002	-	4,4,4	0.24	0	6,6,6	0.09	0
3	HR2	D	3004	-	40,41,41	1.22	5 (12%)	42,58,58	1.34	3 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	2003	-	4,4,4	0.22	0	6,6,6	0.18	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	HR2	A	3001	-	-	3/25/39/39	0/4/4/4
3	HR2	C	3003	-	-	3/25/39/39	0/4/4/4
3	HR2	A	3002	-	-	2/25/39/39	0/4/4/4
3	HR2	D	3004	-	-	3/25/39/39	0/4/4/4

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3003	HR2	O27-C25	3.58	1.33	1.22
3	A	3001	HR2	O27-C25	3.54	1.33	1.22
3	D	3004	HR2	O27-C25	3.54	1.33	1.22
3	A	3002	HR2	O27-C25	3.50	1.33	1.22
3	A	3002	HR2	C17-N15	-3.47	1.36	1.43
3	D	3004	HR2	C17-N15	-3.40	1.36	1.43
3	C	3003	HR2	C17-N15	-3.37	1.36	1.43
3	A	3001	HR2	C17-N15	-3.22	1.37	1.43
3	C	3003	HR2	O26-C25	-2.62	1.22	1.30
3	A	3001	HR2	O26-C25	-2.59	1.22	1.30
3	D	3004	HR2	O26-C25	-2.56	1.22	1.30
3	A	3002	HR2	O26-C25	-2.51	1.22	1.30
3	D	3004	HR2	C1-N1	-2.47	1.35	1.41
3	A	3002	HR2	C1-N1	-2.42	1.35	1.41
3	A	3001	HR2	C1-N1	-2.37	1.35	1.41
3	C	3003	HR2	C1-N1	-2.37	1.35	1.41
3	C	3003	HR2	C13-N15	-2.29	1.34	1.40
3	A	3001	HR2	C13-N15	-2.28	1.34	1.40
3	D	3004	HR2	C13-N15	-2.28	1.34	1.40
3	A	3002	HR2	C13-N15	-2.27	1.34	1.40

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3003	HR2	C13-C1-C4	-4.25	117.93	133.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3004	HR2	C13-C1-C4	-4.24	117.96	133.09
3	A	3002	HR2	C13-C1-C4	-4.24	117.99	133.09
3	A	3001	HR2	C13-C1-C4	-4.21	118.08	133.09
3	D	3004	HR2	C20-C19-C3	-3.46	106.28	113.36
3	A	3002	HR2	C20-C19-C3	-2.63	107.98	113.36
3	A	3001	HR2	C20-C19-C3	-2.38	108.49	113.36
3	A	3001	HR2	C18-C7-C15	-2.22	119.88	122.80
3	A	3002	HR2	C18-C7-C15	-2.20	119.92	122.80
3	C	3003	HR2	C22-C23-C24	-2.09	108.70	112.96
3	C	3003	HR2	C19-C20-C21	-2.08	109.66	113.58
3	C	3003	HR2	C18-C7-C15	-2.05	120.11	122.80
3	D	3004	HR2	C18-C7-C15	-2.01	120.17	122.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3001	HR2	C32-C17-N15-C16
3	A	3002	HR2	C28-C17-N15-C16
3	A	3002	HR2	C32-C17-N15-C16
3	C	3003	HR2	C32-C17-N15-C16
3	C	3003	HR2	C19-C20-C21-O33
3	C	3003	HR2	C19-C20-C21-C22
3	A	3001	HR2	C19-C20-C21-O33
3	D	3004	HR2	C19-C20-C21-O33
3	A	3001	HR2	C28-C17-N15-C16
3	D	3004	HR2	C28-C17-N15-C16
3	D	3004	HR2	C32-C17-N15-C16

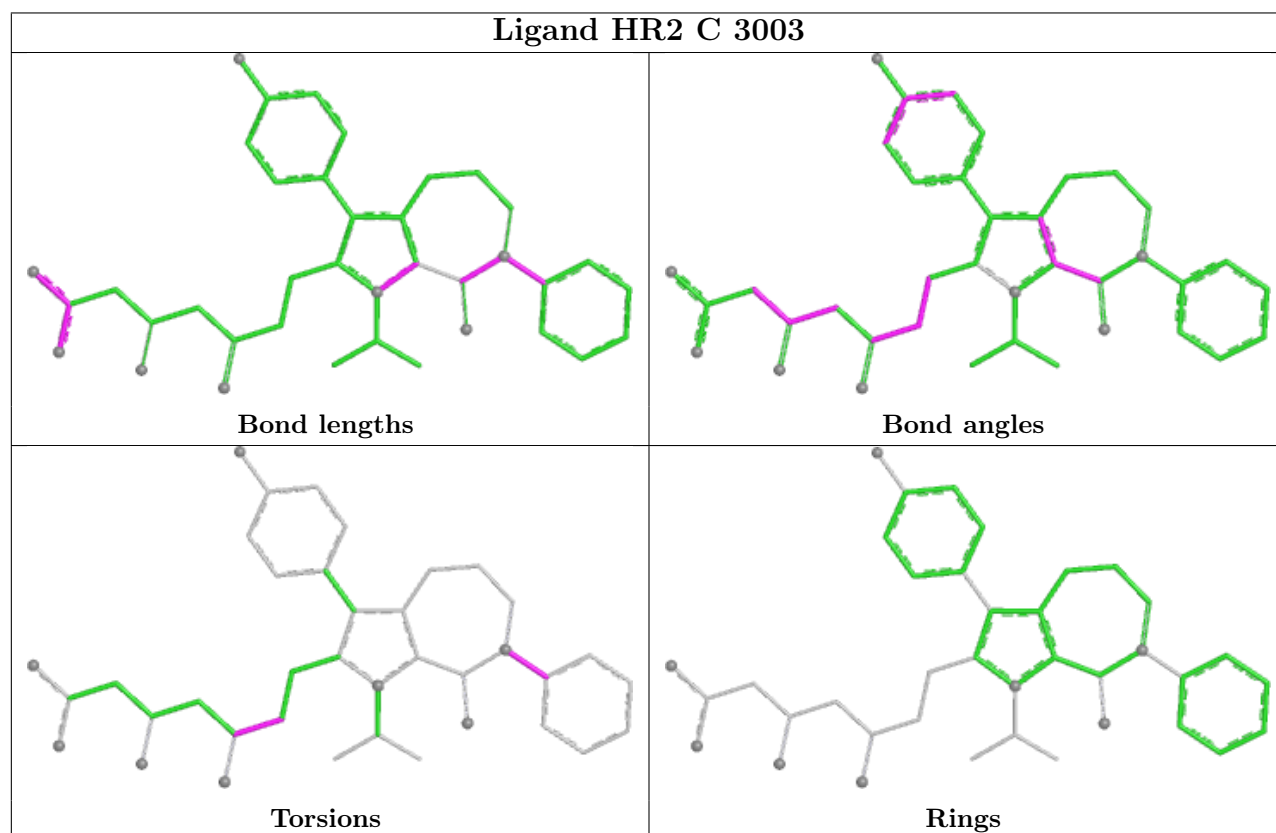
There are no ring outliers.

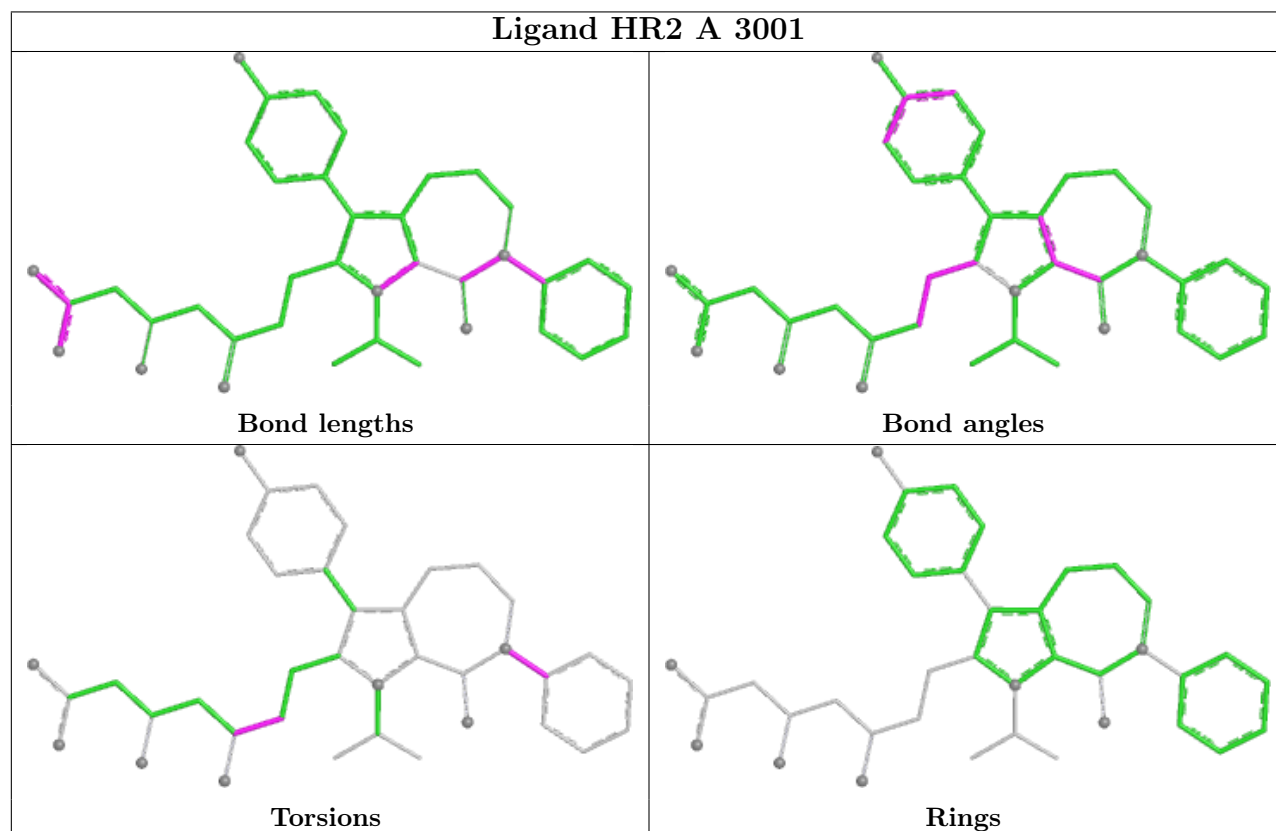
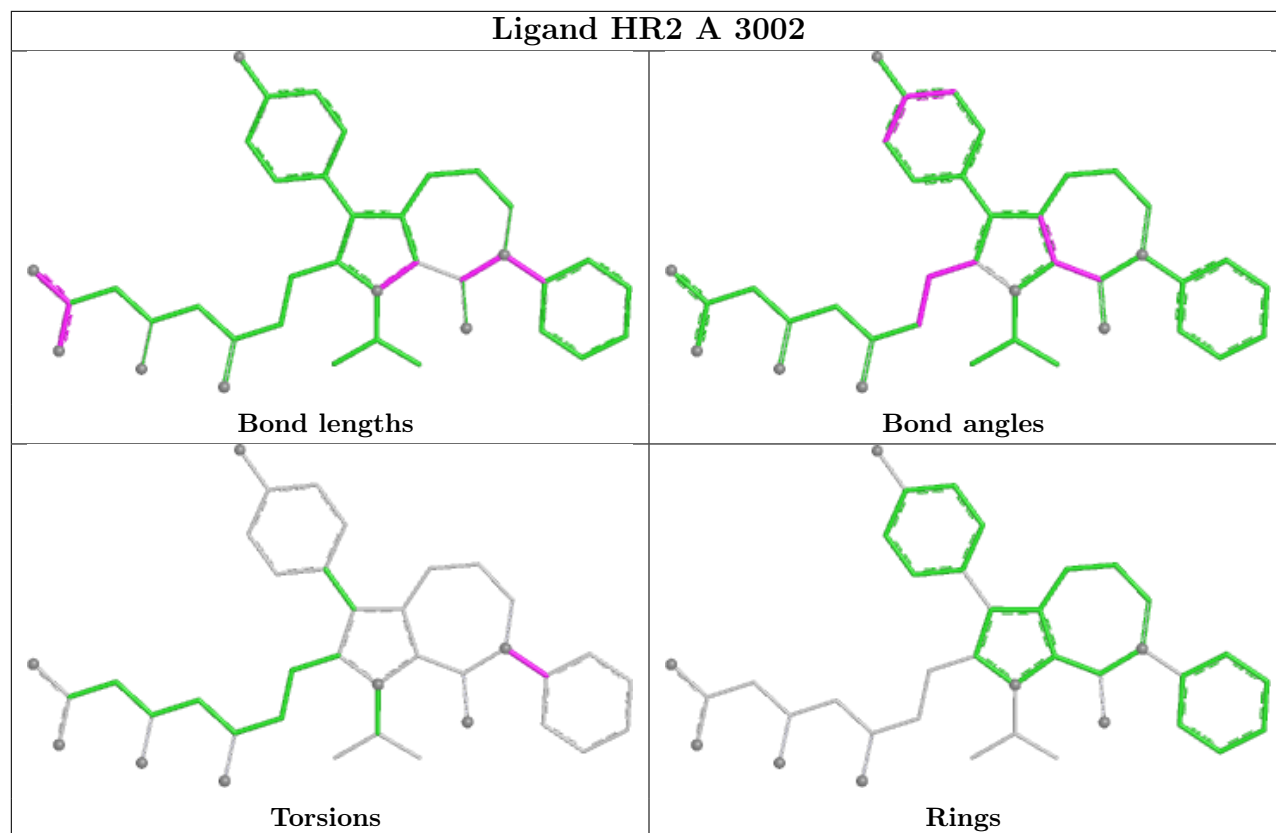
2 monomers are involved in 2 short contacts:

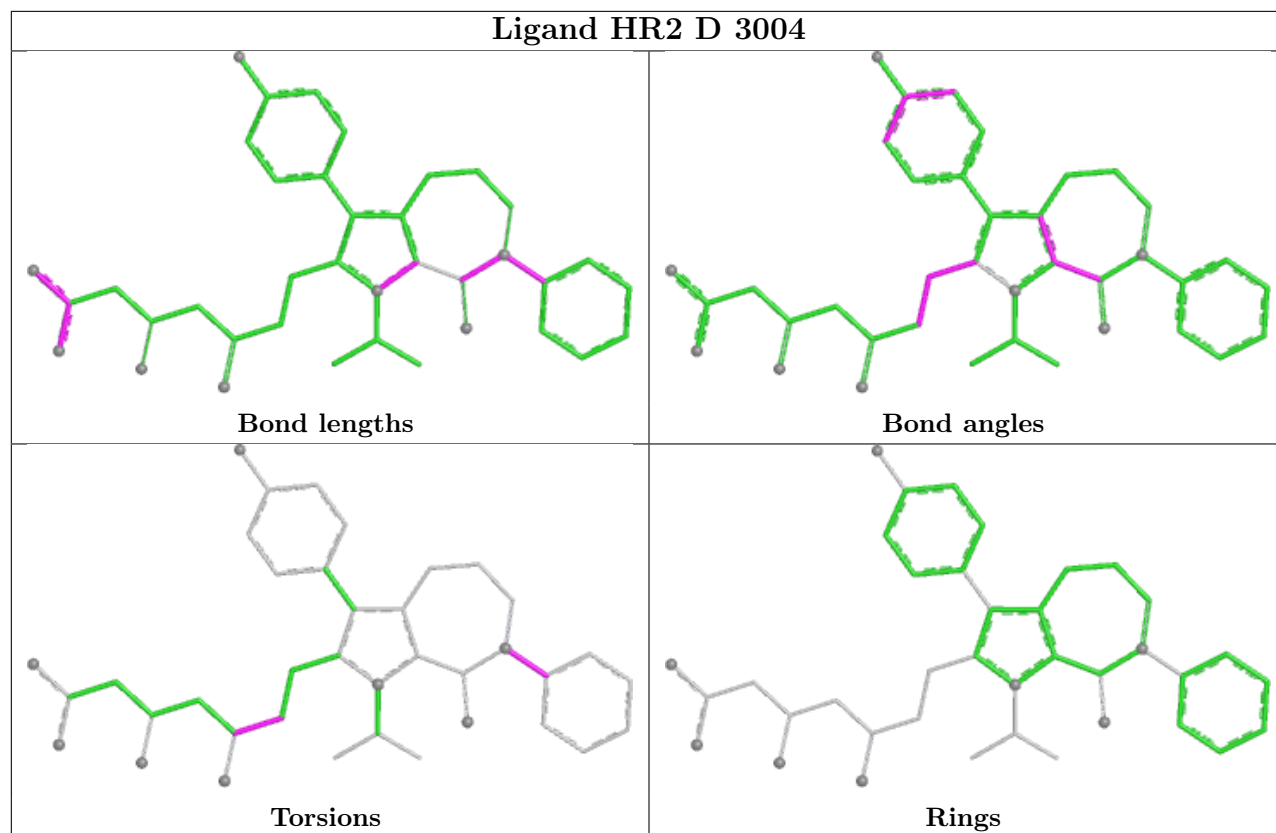
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3003	HR2	1	0
3	D	3004	HR2	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	425/441 (96%)	1.33	91 (21%) 2 2	20, 29, 52, 63	0
1	B	423/441 (95%)	1.37	85 (20%) 3 2	18, 28, 58, 60	0
1	C	422/441 (95%)	1.17	65 (15%) 5 4	19, 28, 40, 57	0
1	D	418/441 (94%)	1.23	84 (20%) 3 2	17, 28, 56, 61	0
All	All	1688/1764 (95%)	1.28	325 (19%) 3 3	17, 28, 55, 63	0

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	483	THR	6.2
1	A	458	GLY	6.1
1	B	479	TYR	5.8
1	A	459	ALA	5.6
1	B	473	ALA	5.6
1	C	476	ILE	5.6
1	C	477	PRO	5.5
1	A	478	ALA	5.3
1	B	511	TYR	5.3
1	C	861	HIS	5.3
1	B	483	THR	5.3
1	B	477	PRO	5.2
1	B	461	PHE	5.2
1	B	449	LEU	5.2
1	D	449	LEU	5.2
1	D	470	LEU	5.1
1	C	483	THR	5.1
1	C	455	ALA	5.0
1	D	478	ALA	5.0
1	A	477	PRO	4.9
1	B	470	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	481	LEU	4.9
1	B	451	ILE	4.8
1	D	476	ILE	4.8
1	A	574	GLY	4.8
1	C	479	TYR	4.7
1	D	629	ALA	4.7
1	C	475	HIS	4.6
1	B	463	SER	4.6
1	B	450	GLN	4.5
1	B	476	ILE	4.5
1	A	463	SER	4.4
1	D	473	ALA	4.4
1	B	442	PRO	4.4
1	A	479	TYR	4.3
1	C	484	LEU	4.3
1	D	442	PRO	4.3
1	D	484	LEU	4.2
1	B	485	ILE	4.2
1	B	455	ALA	4.2
1	A	446	GLU	4.2
1	B	487	THR	4.2
1	A	453	GLY	4.1
1	A	442	PRO	4.1
1	D	465	ALA	4.0
1	D	464	ASP	4.0
1	B	465	ALA	4.0
1	D	479	TYR	4.0
1	B	469	GLN	4.0
1	A	467	ILE	4.0
1	D	468	ILE	3.9
1	D	482	GLU	3.9
1	B	626	SER	3.9
1	B	786	PRO	3.9
1	A	468	ILE	3.9
1	C	474	LYS	3.9
1	A	455	ALA	3.8
1	B	863	VAL	3.8
1	D	461	PHE	3.8
1	A	476	ILE	3.7
1	A	494	ILE	3.7
1	C	488	HIS	3.7
1	A	503	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	484	LEU	3.7
1	A	481	LEU	3.6
1	B	452	LEU	3.6
1	B	472	ASN	3.6
1	C	442	PRO	3.6
1	C	862	LEU	3.6
1	A	475	HIS	3.6
1	D	627	ARG	3.6
1	A	445	ASN	3.5
1	B	444	PRO	3.5
1	D	477	PRO	3.5
1	A	452	LEU	3.5
1	D	447	GLU	3.5
1	A	485	ILE	3.5
1	A	470	LEU	3.5
1	C	860	GLY	3.5
1	B	447	GLU	3.5
1	A	454	ASN	3.5
1	B	499	LEU	3.5
1	B	503	LEU	3.5
1	D	460	LYS	3.5
1	B	506	PRO	3.4
1	D	459	ALA	3.4
1	D	462	LEU	3.4
1	D	496	ARG	3.4
1	B	445	ASN	3.4
1	D	483	THR	3.4
1	D	458	GLY	3.4
1	D	487	THR	3.4
1	D	787	THR	3.4
1	B	627	ARG	3.4
1	B	486	GLU	3.4
1	B	481	LEU	3.4
1	B	448	CYS	3.3
1	B	630	ARG	3.3
1	B	457	LYS	3.3
1	B	829	ASP	3.3
1	C	478	ALA	3.3
1	C	657	MET	3.3
1	B	491	GLY	3.2
1	A	457	LYS	3.2
1	A	473	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	829	ASP	3.2
1	A	637	SER	3.2
1	D	486	GLU	3.2
1	C	863	VAL	3.1
1	D	630	ARG	3.1
1	B	468	ILE	3.1
1	A	487	THR	3.1
1	C	454	ASN	3.1
1	B	509	LEU	3.1
1	C	481	LEU	3.1
1	A	715	LYS	3.1
1	C	626	SER	3.1
1	A	717	VAL	3.1
1	B	467	ILE	3.1
1	D	620	GLU	3.0
1	A	633	LYS	3.0
1	C	500	SER	3.0
1	B	480	LYS	3.0
1	D	475	HIS	3.0
1	D	626	SER	3.0
1	D	771	ASN	3.0
1	B	475	HIS	3.0
1	D	472	ASN	3.0
1	A	786	PRO	3.0
1	B	598	ARG	2.9
1	A	482	GLU	2.9
1	B	478	ALA	2.9
1	B	453	GLY	2.9
1	C	600	CYS	2.9
1	D	516	ASP	2.9
1	A	498	LEU	2.9
1	B	498	LEU	2.9
1	A	448	CYS	2.9
1	A	443	ARG	2.9
1	D	485	ILE	2.9
1	B	441	GLU	2.8
1	D	480	LYS	2.8
1	D	450	GLN	2.8
1	D	866	HIS	2.8
1	A	541	ALA	2.8
1	C	471	VAL	2.8
1	B	500	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	507	SER	2.8
1	D	518	ASN	2.8
1	A	450	GLN	2.8
1	A	714	ALA	2.8
1	A	484	LEU	2.8
1	C	633	LYS	2.8
1	D	445	ASN	2.8
1	C	630	ARG	2.8
1	A	787	THR	2.8
1	A	451	ILE	2.8
1	D	628	PHE	2.7
1	A	461	PHE	2.7
1	C	473	ALA	2.7
1	A	506	PRO	2.7
1	A	471	VAL	2.7
1	C	482	GLU	2.7
1	D	657	MET	2.7
1	C	504	SER	2.7
1	C	453	GLY	2.7
1	B	443	ARG	2.7
1	C	857	LEU	2.7
1	A	771	ASN	2.7
1	D	471	VAL	2.7
1	B	524	GLY	2.7
1	A	567	ASN	2.6
1	A	658	ASN	2.6
1	B	521	LEU	2.6
1	A	580	SER	2.6
1	B	514	TYR	2.6
1	A	474	LYS	2.6
1	D	600	CYS	2.6
1	C	560	GLY	2.6
1	C	486	GLU	2.6
1	C	727	ALA	2.6
1	D	616	ALA	2.6
1	A	480	LYS	2.6
1	C	829	ASP	2.6
1	D	494	ILE	2.6
1	B	458	GLY	2.6
1	A	727	ALA	2.6
1	B	660	ILE	2.6
1	A	582	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	724	THR	2.6
1	C	859	ALA	2.6
1	C	516	ASP	2.6
1	D	598	ARG	2.6
1	D	723	THR	2.6
1	C	452	LEU	2.6
1	D	469	GLN	2.5
1	C	726	GLU	2.5
1	D	785	GLY	2.5
1	B	816	ALA	2.5
1	D	714	ALA	2.5
1	C	660	ILE	2.5
1	C	526	CYS	2.5
1	A	516	ASP	2.5
1	A	831	PRO	2.5
1	B	462	LEU	2.5
1	A	729	ILE	2.5
1	C	547	ASP	2.5
1	C	730	GLU	2.5
1	D	500	SER	2.5
1	D	865	SER	2.5
1	A	828	LYS	2.5
1	A	861	HIS	2.5
1	B	464	ASP	2.4
1	C	708	CYS	2.4
1	C	792	TYR	2.4
1	A	784	SER	2.4
1	D	463	SER	2.4
1	D	624	SER	2.4
1	A	657	MET	2.4
1	B	639	ALA	2.4
1	B	714	ALA	2.4
1	A	542	GLY	2.4
1	A	788	ASN	2.4
1	C	548	GLU	2.4
1	B	471	VAL	2.4
1	C	522	VAL	2.4
1	A	444	PRO	2.4
1	D	491	GLY	2.4
1	A	464	ASP	2.4
1	C	716	VAL	2.4
1	D	467	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	495	ARG	2.4
1	B	787	THR	2.4
1	A	710	ALA	2.4
1	C	584	LEU	2.4
1	D	505	GLU	2.4
1	A	472	ASN	2.4
1	C	524	GLY	2.4
1	C	771	ASN	2.4
1	D	830	ASN	2.4
1	D	508	SER	2.4
1	B	861	HIS	2.4
1	D	488	HIS	2.4
1	D	634	LEU	2.3
1	D	443	ARG	2.3
1	B	488	HIS	2.3
1	A	441	GLU	2.3
1	D	446	GLU	2.3
1	D	510	GLN	2.3
1	B	525	ALA	2.3
1	A	462	LEU	2.3
1	D	507	SER	2.3
1	B	529	ASN	2.3
1	B	587	GLY	2.3
1	B	860	GLY	2.3
1	C	503	LEU	2.3
1	A	460	LYS	2.3
1	D	828	LYS	2.3
1	A	469	GLN	2.2
1	B	775	SER	2.2
1	D	504	SER	2.2
1	B	492	VAL	2.2
1	A	832	GLY	2.2
1	C	822	GLY	2.2
1	A	791	LEU	2.2
1	B	546	LEU	2.2
1	C	672	HIS	2.2
1	D	632	GLN	2.2
1	C	612	SER	2.2
1	D	676	PRO	2.2
1	A	465	ALA	2.2
1	C	667	ALA	2.2
1	D	448	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	665	GLU	2.2
1	D	782	GLU	2.2
1	A	511	TYR	2.2
1	B	504	SER	2.2
1	B	490	ARG	2.2
1	B	501	LYS	2.2
1	A	820	MET	2.2
1	D	444	PRO	2.2
1	B	547	ASP	2.2
1	A	548	GLU	2.2
1	A	773	GLY	2.2
1	D	784	SER	2.2
1	B	494	ILE	2.1
1	C	451	ILE	2.1
1	A	497	GLN	2.1
1	C	785	GLY	2.1
1	C	572	ALA	2.1
1	D	541	ALA	2.1
1	B	515	ARG	2.1
1	C	449	LEU	2.1
1	C	496	ARG	2.1
1	D	490	ARG	2.1
1	A	456	GLU	2.1
1	D	675	PHE	2.1
1	B	574	GLY	2.1
1	A	812	LEU	2.1
1	A	862	LEU	2.1
1	C	637	SER	2.1
1	A	785	GLY	2.1
1	C	485	ILE	2.1
1	A	629	ALA	2.1
1	C	465	ALA	2.1
1	A	449	LEU	2.1
1	C	669	SER	2.1
1	B	676	PRO	2.1
1	A	660	ILE	2.1
1	C	480	LYS	2.1
1	A	620	GLU	2.0
1	B	782	GLU	2.0
1	D	585	ALA	2.1
1	A	545	CYS	2.0
1	D	595	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	786	PRO	2.0
1	A	517	TYR	2.0
1	B	633	LYS	2.0
1	B	785	GLY	2.0
1	B	726	GLU	2.0
1	D	863	VAL	2.0
1	D	810	ASN	2.0
1	A	795	CYS	2.0
1	A	827	CYS	2.0
1	C	545	CYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

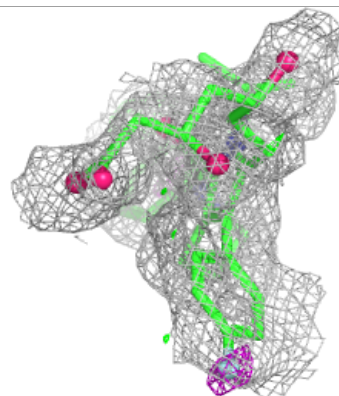
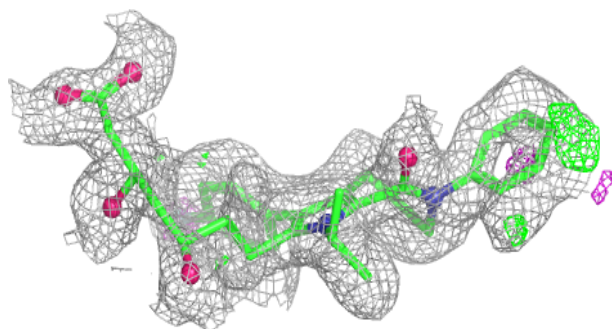
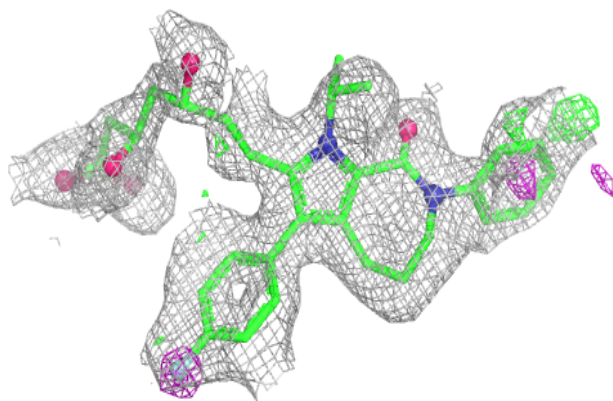
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	2002	5/5	0.75	0.19	63,63,63,63	0
2	SO4	C	2003	5/5	0.80	0.18	46,47,47,47	0
3	HR2	C	3003	38/38	0.81	0.15	28,37,40,42	0
2	SO4	A	2001	5/5	0.84	0.20	53,53,54,54	0
3	HR2	A	3002	38/38	0.86	0.14	28,32,35,37	0
3	HR2	A	3001	38/38	0.86	0.14	27,33,37,38	0
3	HR2	D	3004	38/38	0.86	0.13	24,29,34,36	0
2	SO4	D	2004	5/5	0.88	0.17	44,45,45,45	0

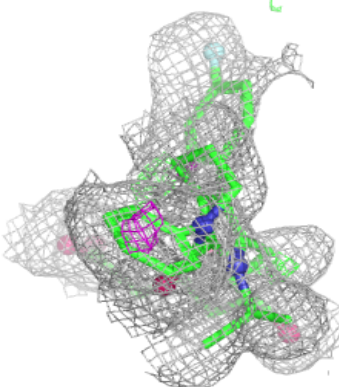
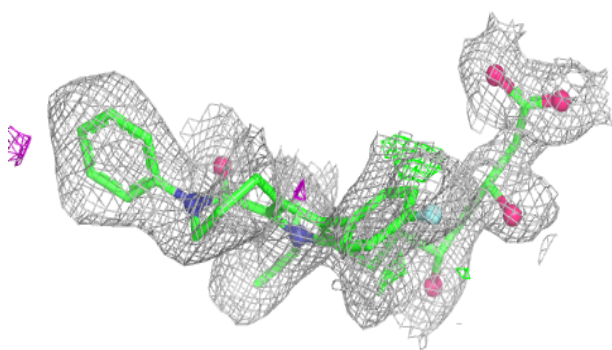
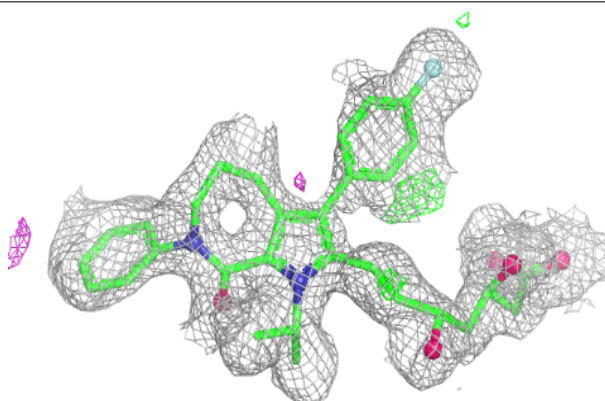
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HR2 C 3003:

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

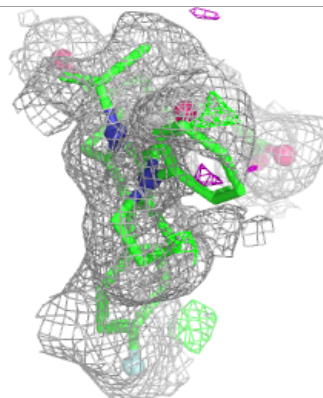
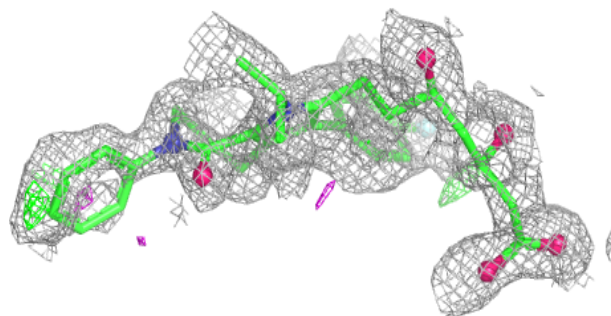
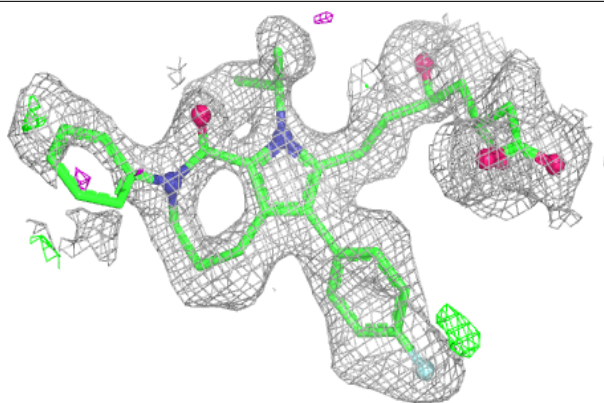
**Electron density around HR2 A 3002:**

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

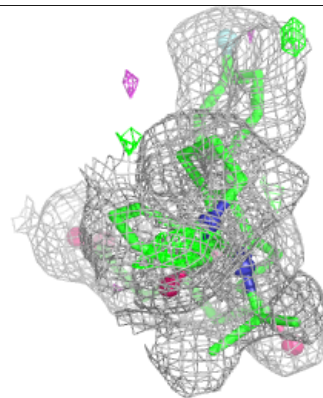
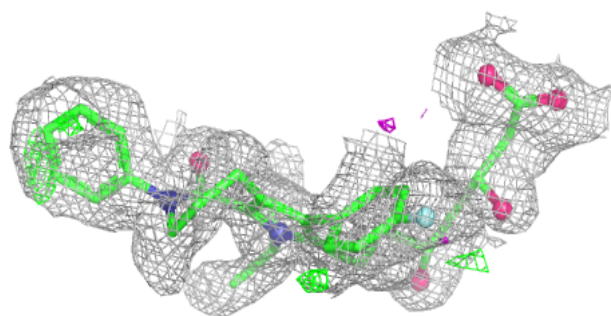
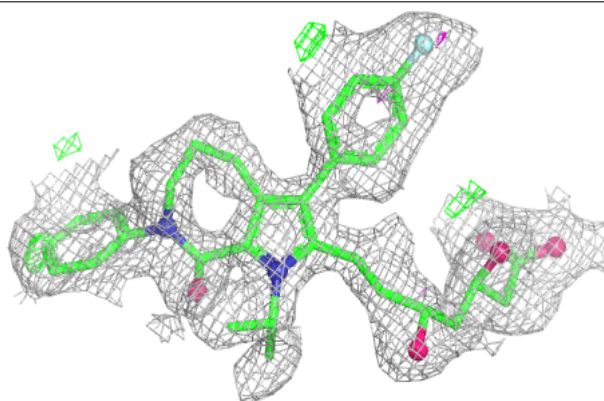


Electron density around HR2 A 3001:

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

**Electron density around HR2 D 3004:**

$2mF_o-DF_c$ (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.