Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:32 AM EDT

PDB ID	:	2Q6C
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)

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

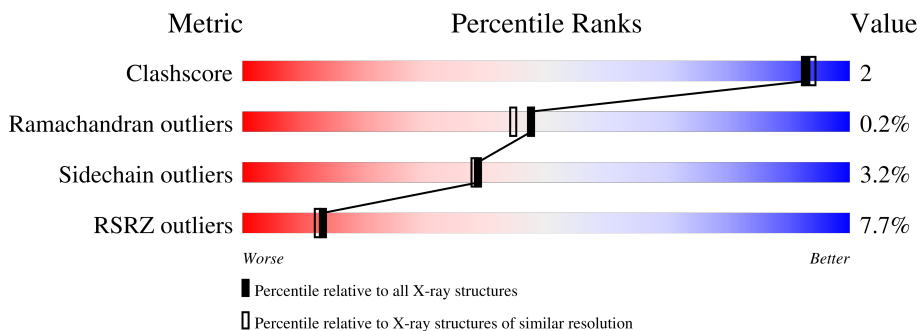|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1   Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
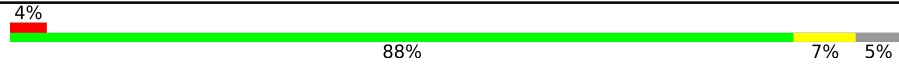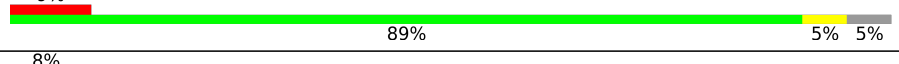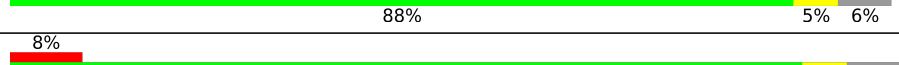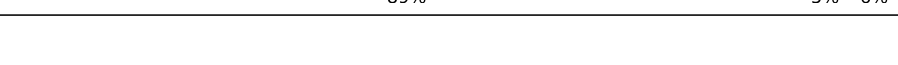*X-RAY DIFFRACTION*

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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		0.2%
Sidechain outliers		3.2%
RSRZ outliers		7.7%

Worse ▯ *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 <=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	4% / 88% / 7% / 5%
1	B	441	9% / 89% / 5% / 5%
1	C	441	8% / 88% / 5% / 6%
1	D	441	8% / 89% / 5% / 6%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 13720 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	421	Total 3133	C 1951	N 551	O 601	S 30	0	6	0
1	B	420	Total 3127	C 1947	N 548	O 602	S 30	0	8	0
1	C	414	Total 3079	C 1918	N 541	O 590	S 30	0	8	0
1	D	413	Total 3077	C 1916	N 541	O 590	S 30	0	6	0

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 (three-letter code: SO4) (formula: O_4S).

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

- Molecule 3 is (3R,5R)-7-[1-(4-FLUOROPHENYL)-3-ISOPROPYL-4-OXO-5-PHENYL-4,5-DIHYDRO-3H-PYRROLO[2,3-C]QUINOLIN-2-YL]-3,5-DIHYDROXYHEPTANOIC ACID (three-letter code: HR1) (formula: $C_{33}H_{33}FN_2O_5$).
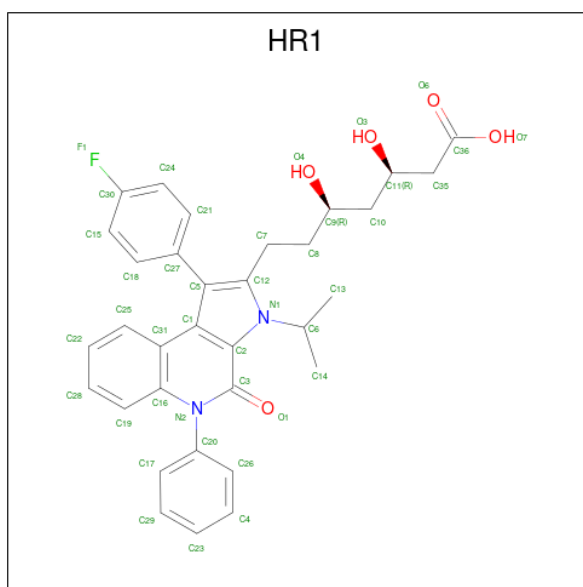
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	B	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	C	1	Total	C	F	N	O	0	0
			41	33	1	2	5		
3	D	1	Total	C	F	N	O	0	0
			41	33	1	2	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	253	Total	O	0	0
			253	253		
4	B	295	Total	O	0	0
			295	295		
4	C	282	Total	O	0	0
			282	282		
4	D	290	Total	O	0	0
			290	290		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain A:

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

Chain B:

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

Chain C:

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

Chain D:

HIS HIS HIS HIS HIS GLU P442 R443 P444 N445 E446 E447 C448 L449 Q450 ILE LEU GLY ASN ALA GLU LYS G458 A459 K460 F461 L462 S463 D464 A465 E466 I467 I468 Q469 L470 V471 N472 A473 K474 H475 I476 P477 A478 Y479 K480 L481 E482 T483 L484 I485 E486 T487 H488 Q510 Y514 R515 D516

D547 R595 D623 R627 N642 D690 R702 V731 G765 I793 S799 Q814 D829 L851 H861 LEU VAL LYS SER HIS MET ILE HIS ASN ARG SER LYS ILE ASN

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.82Å 135.37Å 83.12Å 90.00° 97.02° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 41.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.00) 92.1 (41.10-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.18 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.252 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 23.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.090 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13720	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HR1, 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	0.27	0/3179	0.57	7/4298 (0.2%)
1	B	0.27	0/3177	0.56	6/4295 (0.1%)
1	C	0.27	0/3127	0.56	5/4225 (0.1%)
1	D	0.27	0/3127	0.57	5/4226 (0.1%)
All	All	0.27	0/12610	0.57	23/17044 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	547	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	547	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	547	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	690	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	790	ASP	CB-CG-OD2	5.45	123.21	118.30
1	D	623	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	623	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	623	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	653	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	547	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	690	ASP	CB-CG-OD2	5.27	123.05	118.30
1	C	790	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	790	ASP	CB-CG-OD2	5.26	123.03	118.30
1	B	601	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	690	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	829	ASP	CB-CG-OD2	5.17	122.96	118.30
1	D	516	ASP	CB-CG-OD2	5.17	122.96	118.30
1	C	516	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	516	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	829	ASP	CB-CG-OD2	5.11	122.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	601	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	829	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	653	ASP	CB-CG-OD2	5.02	122.82	118.30

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	3133	0	3155	5	0
1	B	3127	0	3148	11	0
1	C	3079	0	3105	7	0
1	D	3077	0	3098	7	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	41	0	32	4	0
3	B	41	0	32	2	0
3	C	41	0	32	3	0
3	D	41	0	32	3	0
4	A	253	0	0	0	0
4	B	295	0	0	0	0
4	C	282	0	0	0	0
4	D	290	0	0	0	0
All	All	13720	0	12634	39	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 2.

All (39) 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:635:HIS:HE2	1:B:696:ILE:HD11	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:HIS:ND1	1:B:635:HIS:C	2.43	0.71
3:A:3002:HR1:H71	3:A:3002:HR1:H133	1.74	0.69
1:C:655:MET:SD	1:C:657[A]:MET:HG3	2.35	0.67
3:B:3001:HR1:H72	3:B:3001:HR1:H133	1.77	0.67
1:C:681:LEU:HD22	1:D:731:VAL:HG22	1.80	0.63
1:B:635:HIS:NE2	1:B:696:ILE:HD11	2.16	0.59
3:B:3001:HR1:H142	3:B:3001:HR1:H82	1.88	0.56
3:A:3002:HR1:H142	3:A:3002:HR1:H72	1.92	0.51
1:A:657[A]:MET:HE1	1:A:702:ARG:HH22	1.76	0.50
1:C:793:ILE:HD13	1:C:851:LEU:HG	1.95	0.49
1:D:595:ARG:HE	1:D:642:ASN:HD21	1.62	0.48
3:D:3003:HR1:H25	3:D:3003:HR1:C18	2.43	0.48
3:C:3004:HR1:H71	3:C:3004:HR1:H133	1.95	0.48
1:D:702:ARG:O	1:D:799:SER:HA	2.15	0.46
3:C:3004:HR1:H25	3:C:3004:HR1:C18	2.46	0.46
1:D:642:ASN:HD22	1:D:642:ASN:N	2.14	0.46
1:D:595:ARG:HE	1:D:642:ASN:ND2	2.14	0.45
1:C:774:SER:HA	1:C:799:SER:O	2.17	0.44
1:A:449:LEU:HD11	1:A:475:HIS:CD2	2.52	0.44
1:B:702:ARG:O	1:B:799:SER:HA	2.17	0.44
1:B:793:ILE:HD13	1:B:851:LEU:HG	2.00	0.44
1:C:635:HIS:HB3	1:C:646:ARG:HB3	2.00	0.43
1:A:619:LYS:HZ1	1:A:630[A]:ARG:CD	2.32	0.43
1:A:793:ILE:HD13	1:A:851:LEU:HG	2.01	0.43
3:D:3003:HR1:H71	3:D:3003:HR1:H133	2.01	0.42
1:C:702:ARG:O	1:C:799:SER:HA	2.20	0.42
1:A:702:ARG:O	1:A:799:SER:HA	2.20	0.42
1:B:657[A]:MET:HE1	1:B:690:ASP:CG	2.40	0.42
3:D:3003:HR1:H71	3:D:3003:HR1:H142	2.02	0.41
3:A:3002:HR1:H25	3:A:3002:HR1:C27	2.51	0.41
1:D:793:ILE:HD13	1:D:851:LEU:HG	2.03	0.41
1:B:441:GLU:N	1:B:442:PRO:CD	2.84	0.41
1:B:635:HIS:ND1	1:B:635:HIS:O	2.54	0.40
3:A:3002:HR1:H21	1:B:853:LEU:HD11	2.03	0.40
1:B:669:SER:O	1:B:672:HIS:HB2	2.21	0.40
3:C:3004:HR1:H71	3:C:3004:HR1:H142	2.02	0.40
1:B:796:THR:HG21	1:C:638:ILE:O	2.22	0.40
1:D:765:GLY:CA	1:D:814:GLN:HG2	2.51	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	419/441 (95%)	405 (97%)	14 (3%)	0	100	100
1	B	419/441 (95%)	404 (96%)	14 (3%)	1 (0%)	47	44
1	C	411/441 (93%)	395 (96%)	15 (4%)	1 (0%)	47	44
1	D	410/441 (93%)	396 (97%)	13 (3%)	1 (0%)	47	44
All	All	1659/1764 (94%)	1600 (96%)	56 (3%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	474	LYS
1	B	514	TYR
1	D	514	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	335/355 (94%)	318 (95%)	17 (5%)	24	19
1	B	335/355 (94%)	328 (98%)	7 (2%)	53	57
1	C	330/355 (93%)	319 (97%)	11 (3%)	38	37
1	D	330/355 (93%)	323 (98%)	7 (2%)	53	57
All	All	1330/1420 (94%)	1288 (97%)	42 (3%)	39	38

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	ARG
1	A	447	GLU
1	A	449	LEU
1	A	469	GLN
1	A	474	LYS
1	A	484	LEU
1	A	498	LEU
1	A	512	LEU
1	A	523	MET
1	A	634	LEU
1	A	637	SER
1	A	677	GLU
1	A	688	CYS
1	A	752	HIS
1	A	771[A]	ASN
1	A	788	ASN
1	A	814	GLN
1	B	486	GLU
1	B	488	HIS
1	B	505	GLU
1	B	523	MET
1	B	630[A]	ARG
1	B	635	HIS
1	B	728	MET
1	C	452	LEU
1	C	469	GLN
1	C	475	HIS
1	C	490	ARG
1	C	500	SER
1	C	626	SER
1	C	657[A]	MET
1	C	666	LYS
1	C	681	LEU
1	C	771[A]	ASN
1	C	828	LYS
1	D	446	GLU
1	D	450	GLN
1	D	466	GLU
1	D	484	LEU
1	D	486	GLU
1	D	487	THR
1	D	510	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	510	GLN
1	A	518	ASN
1	A	567	ASN
1	A	771[A]	ASN
1	A	788	ASN
1	B	472	ASN
1	B	510	GLN
1	B	529	ASN
1	B	635	HIS
1	C	672	HIS
1	C	679	GLN
1	C	771[A]	ASN
1	D	518	ASN
1	D	642	ASN
1	D	861	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
3	HR1	D	3003	-	40,45,45	1.27	4 (10%)	48,65,65	1.87	7 (14%)
3	HR1	C	3004	-	40,45,45	1.30	4 (10%)	48,65,65	1.79	6 (12%)
2	SO4	C	2003	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	A	2001	-	4,4,4	0.16	0	6,6,6	0.11	0
2	SO4	B	2002	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	D	2004	-	4,4,4	0.15	0	6,6,6	0.13	0
3	HR1	B	3001	-	40,45,45	1.20	3 (7%)	48,65,65	2.12	10 (20%)
3	HR1	A	3002	-	40,45,45	1.31	4 (10%)	48,65,65	1.80	6 (12%)

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	HR1	D	3003	-	-	4/23/25/25	0/5/5/5
3	HR1	C	3004	-	-	6/23/25/25	0/5/5/5
3	HR1	A	3002	-	-	9/23/25/25	0/5/5/5
3	HR1	B	3001	-	-	4/23/25/25	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3002	HR1	C5-C12	5.30	1.50	1.40
3	C	3004	HR1	C5-C12	5.01	1.49	1.40
3	D	3003	HR1	C5-C12	4.84	1.49	1.40
3	B	3001	HR1	C5-C12	4.49	1.48	1.40
3	D	3003	HR1	C1-C2	3.29	1.46	1.42
3	C	3004	HR1	C1-C2	3.25	1.46	1.42
3	B	3001	HR1	C1-C2	3.19	1.46	1.42
3	A	3002	HR1	C1-C2	3.14	1.46	1.42
3	D	3003	HR1	C20-N2	-2.91	1.42	1.45
3	C	3004	HR1	C20-N2	-2.91	1.42	1.45
3	A	3002	HR1	C20-N2	-2.81	1.42	1.45
3	B	3001	HR1	C20-N2	-2.73	1.42	1.45
3	C	3004	HR1	C5-C1	2.17	1.46	1.43
3	D	3003	HR1	C5-C1	2.08	1.46	1.43
3	A	3002	HR1	C5-C1	2.05	1.46	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	3001	HR1	C3-C2-C1	-9.61	113.79	119.96
3	D	3003	HR1	C3-C2-C1	-9.55	113.83	119.96
3	A	3002	HR1	C3-C2-C1	-9.29	114.00	119.96
3	C	3004	HR1	C3-C2-C1	-9.22	114.04	119.96
3	B	3001	HR1	C7-C12-C5	-4.25	123.08	130.34
3	B	3001	HR1	C7-C8-C9	-4.20	106.97	115.05
3	C	3004	HR1	C1-C31-C16	-3.34	116.19	119.29
3	D	3003	HR1	C1-C31-C16	-3.32	116.20	119.29
3	B	3001	HR1	C1-C31-C16	-3.31	116.21	119.29
3	A	3002	HR1	C1-C31-C16	-3.23	116.29	119.29
3	B	3001	HR1	C31-C1-C2	3.01	122.41	119.99
3	D	3003	HR1	C31-C1-C2	2.84	122.27	119.99
3	B	3001	HR1	C25-C31-C16	2.66	121.47	117.80
3	A	3002	HR1	C31-C1-C2	2.60	122.08	119.99
3	C	3004	HR1	C31-C16-N2	2.60	120.64	119.09
3	D	3003	HR1	C31-C16-N2	2.53	120.61	119.09
3	B	3001	HR1	C10-C11-C35	-2.48	108.25	113.19
3	C	3004	HR1	C31-C1-C2	2.44	121.95	119.99
3	B	3001	HR1	C31-C16-N2	2.41	120.54	119.09
3	A	3002	HR1	C31-C16-N2	2.40	120.53	119.09
3	D	3003	HR1	C7-C12-C5	-2.39	126.27	130.34
3	B	3001	HR1	C21-C27-C5	-2.30	117.28	120.77
3	B	3001	HR1	C24-C30-C15	-2.16	119.95	122.83
3	C	3004	HR1	C24-C30-C15	-2.15	119.97	122.83
3	A	3002	HR1	C24-C30-C15	-2.12	120.00	122.83
3	A	3002	HR1	C7-C8-C9	-2.12	110.97	115.05
3	D	3003	HR1	C24-C30-C15	-2.07	120.08	122.83
3	C	3004	HR1	C7-C8-C9	-2.06	111.09	115.05
3	D	3003	HR1	C17-C20-N2	2.06	121.15	119.24

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3002	HR1	C21-C27-C5-C1
3	A	3002	HR1	C18-C27-C5-C1
3	B	3001	HR1	C21-C27-C5-C1
3	B	3001	HR1	C18-C27-C5-C1
3	C	3004	HR1	N1-C12-C7-C8
3	C	3004	HR1	C5-C12-C7-C8
3	D	3003	HR1	C5-C12-C7-C8
3	A	3002	HR1	C7-C8-C9-O4
3	A	3002	HR1	C5-C12-C7-C8

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Mol	Chain	Res	Type	Atoms
3	C	3004	HR1	C18-C27-C5-C1
3	A	3002	HR1	N1-C12-C7-C8
3	D	3003	HR1	N1-C12-C7-C8
3	A	3002	HR1	C18-C27-C5-C12
3	B	3001	HR1	C21-C27-C5-C12
3	B	3001	HR1	C18-C27-C5-C12
3	A	3002	HR1	C21-C27-C5-C12
3	C	3004	HR1	C21-C27-C5-C1
3	A	3002	HR1	C13-C6-N1-C2
3	A	3002	HR1	C14-C6-N1-C2
3	C	3004	HR1	C13-C6-N1-C2
3	C	3004	HR1	C14-C6-N1-C2
3	D	3003	HR1	C13-C6-N1-C2
3	D	3003	HR1	C14-C6-N1-C2

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3003	HR1	3	0
3	C	3004	HR1	3	0
3	B	3001	HR1	2	0
3	A	3002	HR1	4	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 HR1 D 3003

Bond lengths

Bond angles

Torsions

Rings

Ligand HR1 C 3004

Bond lengths

Bond angles

Torsions

Rings

Ligand HR1 B 3001

Bond lengths

Bond angles

Torsions

Rings

Ligand HR1 A 3002

Bond lengths

Bond angles

Torsions

Rings
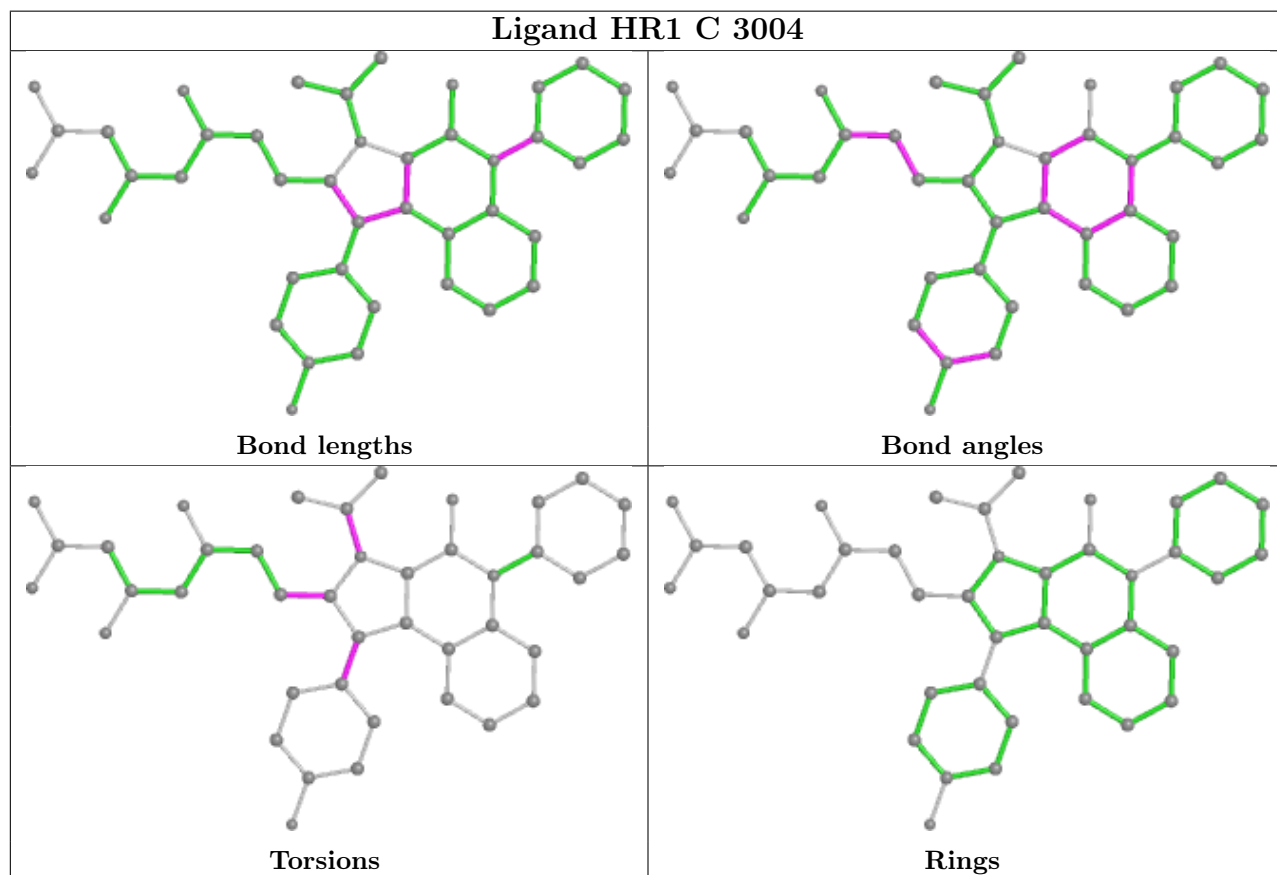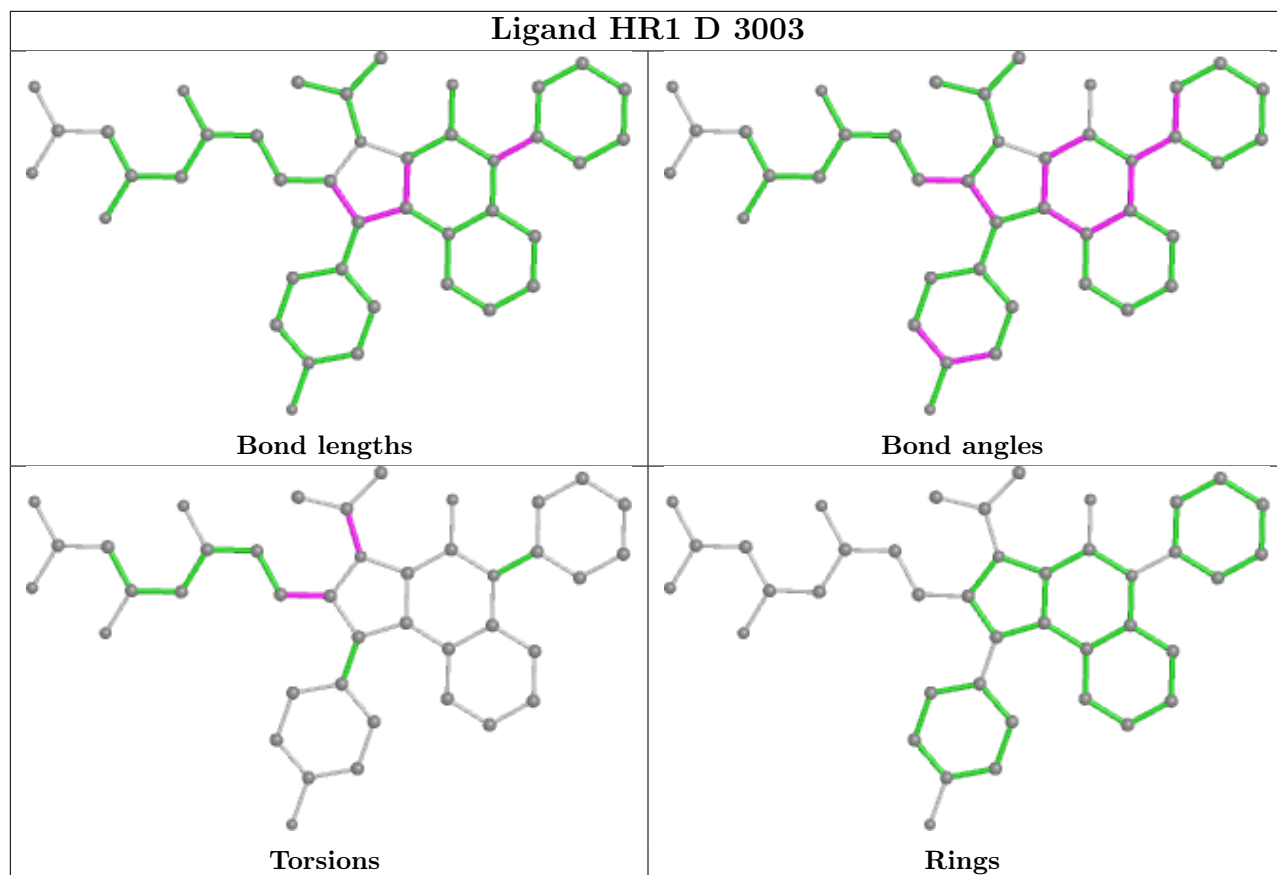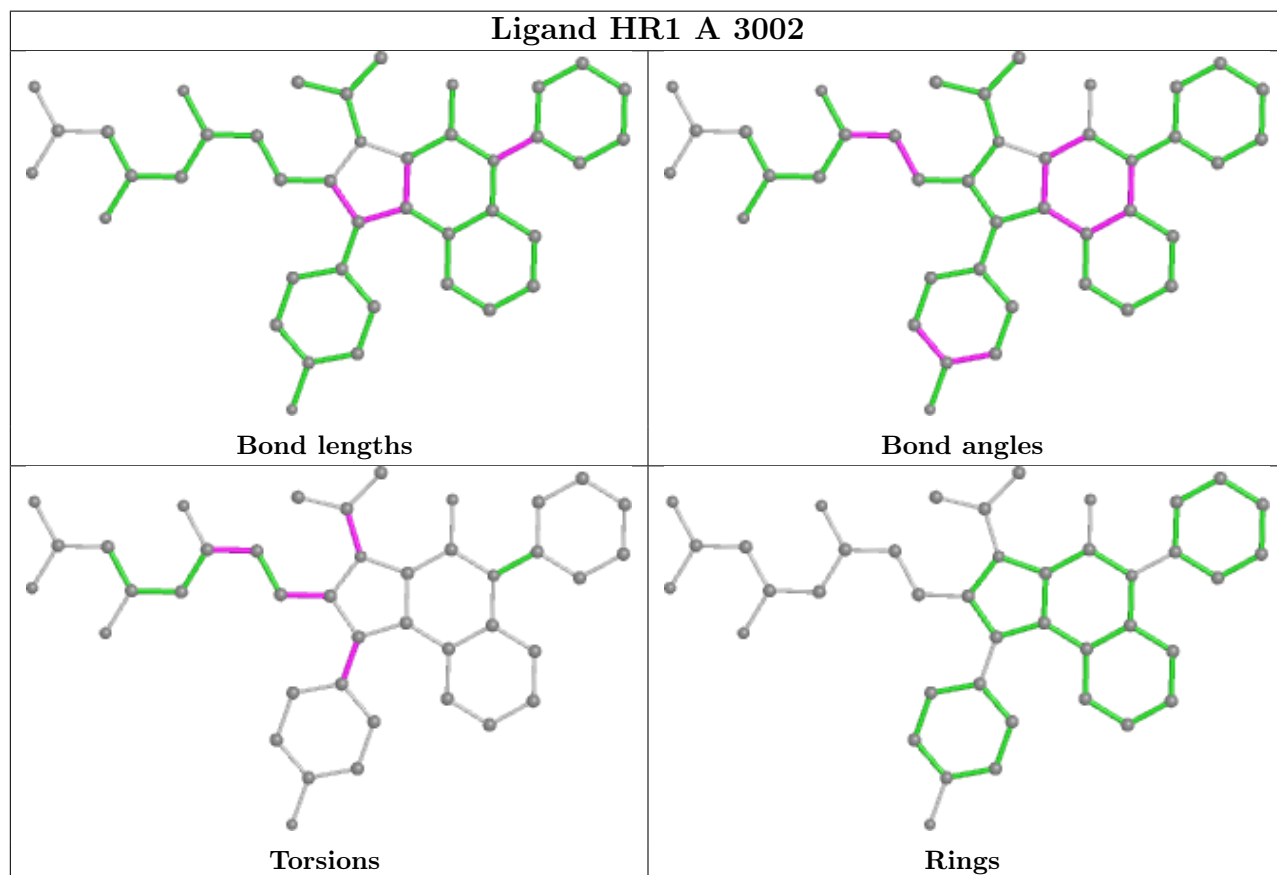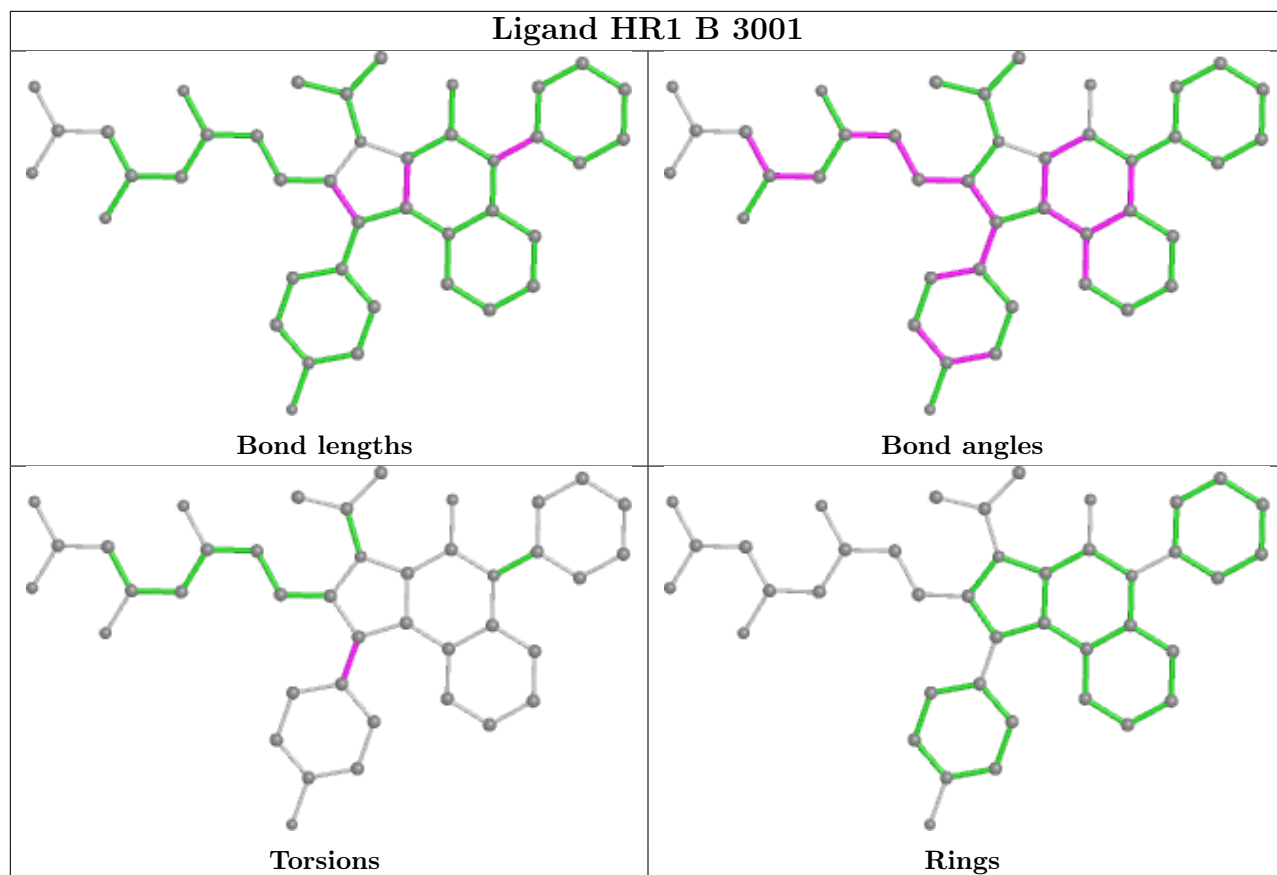
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	421/441 (95%)	0.05	19 (4%)	33	32	16, 27, 50, 55	6 (1%)
1	B	420/441 (95%)	0.36	39 (9%)	8	8	16, 28, 55, 57	6 (1%)
1	C	414/441 (93%)	0.23	35 (8%)	10	10	14, 26, 55, 58	6 (1%)
1	D	413/441 (93%)	0.42	36 (8%)	10	9	16, 26, 55, 58	4 (0%)
All	All	1668/1764 (94%)	0.27	129 (7%)	13	12	14, 27, 55, 58	22 (1%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	481	LEU	21.9
1	D	473	ALA	15.5
1	C	479	TYR	12.8
1	D	476	ILE	12.5
1	D	484	LEU	12.0
1	B	477	PRO	11.8
1	B	479	TYR	11.8
1	B	481	LEU	11.6
1	B	449	LEU	11.6
1	D	480	LYS	11.4
1	B	455	ALA	10.9
1	D	479	TYR	10.6
1	B	461	PHE	10.2
1	C	473	ALA	10.1
1	D	483	THR	10.1
1	D	475	HIS	9.8
1	D	472	ASN	9.7
1	D	446	GLU	9.6
1	D	444	PRO	9.0
1	B	458	GLY	8.9
1	B	480	LYS	8.6

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Mol	Chain	Res	Type	RSRZ
1	B	444	PRO	8.5
1	B	450	GLN	8.2
1	D	458	GLY	8.2
1	A	453	GLY	8.0
1	C	481	LEU	8.0
1	A	455	ALA	8.0
1	B	453	GLY	7.7
1	C	484	LEU	7.4
1	D	468	ILE	7.4
1	C	472	ASN	7.1
1	A	449	LEU	7.1
1	D	470	LEU	7.1
1	B	478	ALA	7.1
1	B	459	ALA	6.6
1	B	452	LEU	6.6
1	D	448	CYS	6.5
1	D	474	LYS	6.5
1	C	461	PHE	6.5
1	C	474	LYS	6.5
1	A	452	LEU	6.3
1	D	477	PRO	6.2
1	B	475	HIS	6.2
1	D	462	LEU	6.1
1	D	478	ALA	6.1
1	A	454	ASN	5.9
1	C	475	HIS	5.8
1	B	445	ASN	5.6
1	A	461	PHE	5.4
1	D	461	PHE	5.3
1	A	441	GLU	5.3
1	C	469	GLN	5.1
1	C	476	ILE	5.0
1	D	469	GLN	5.0
1	B	476	ILE	4.9
1	C	483	THR	4.9
1	D	445	ASN	4.8
1	D	443	ARG	4.8
1	A	450	GLN	4.8
1	C	480	LYS	4.7
1	C	448	CYS	4.7
1	B	474	LYS	4.6
1	C	477	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	457	LYS	4.5
1	B	454	ASN	4.5
1	C	486	GLU	4.5
1	B	483	THR	4.4
1	D	450	GLN	4.4
1	C	454	ASN	4.4
1	C	471	VAL	4.3
1	D	459	ALA	4.3
1	B	473	ALA	4.3
1	B	472	ASN	4.3
1	D	486	GLU	4.2
1	A	456	GLU	4.2
1	B	448	CYS	4.1
1	C	453	GLY	4.1
1	C	452	LEU	4.0
1	D	442	PRO	4.0
1	D	471	VAL	4.0
1	B	672	HIS	4.0
1	C	447	GLU	3.9
1	C	458	GLY	3.9
1	D	463	SER	3.9
1	B	635	HIS	3.9
1	C	450	GLN	3.9
1	D	447	GLU	3.9
1	A	861	HIS	3.8
1	C	446	GLU	3.7
1	B	447	GLU	3.6
1	B	446	GLU	3.6
1	C	465	ALA	3.6
1	B	484	LEU	3.6
1	B	485	ILE	3.5
1	C	444	PRO	3.4
1	B	482	GLU	3.4
1	C	478	ALA	3.4
1	C	468	ILE	3.3
1	B	469	GLN	3.3
1	C	829	ASP	3.3
1	A	458	GLY	3.2
1	A	457	LYS	3.1
1	D	627	ARG	3.1
1	B	441	GLU	3.0
1	A	445	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	462	LEU	2.9
1	C	487	THR	2.8
1	C	470	LEU	2.8
1	B	471	VAL	2.7
1	C	445	ASN	2.7
1	C	482	GLU	2.7
1	D	487	THR	2.7
1	A	672	HIS	2.7
1	B	451	ILE	2.6
1	A	444	PRO	2.5
1	A	442	PRO	2.5
1	D	488	HIS	2.4
1	A	446	GLU	2.4
1	C	633	LYS	2.4
1	C	449	LEU	2.3
1	B	468	ILE	2.3
1	A	462	LEU	2.2
1	C	451	ILE	2.2
1	D	465	ALA	2.2
1	D	861	HIS	2.1
1	B	633	LYS	2.1
1	A	665	GLU	2.1
1	B	456	GLU	2.1
1	D	464	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	A	2001	5/5	0.86	0.17	58,58,58,58	0
3	HR1	B	3001	41/41	0.87	0.16	21,36,39,39	0
3	HR1	A	3002	41/41	0.88	0.17	20,34,37,37	0
3	HR1	C	3004	41/41	0.90	0.14	18,33,35,35	0
2	SO4	B	2002	5/5	0.91	0.17	52,52,52,52	0
3	HR1	D	3003	41/41	0.91	0.13	18,28,31,32	0
2	SO4	D	2004	5/5	0.94	0.12	40,41,41,41	0
2	SO4	C	2003	5/5	0.96	0.10	45,45,45,45	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.
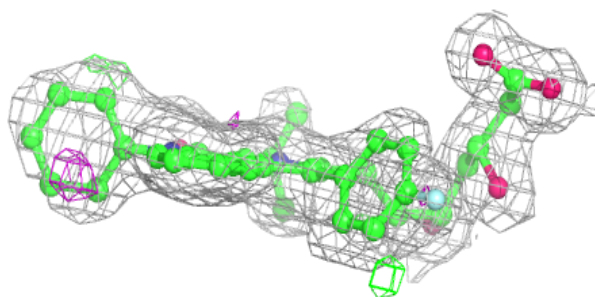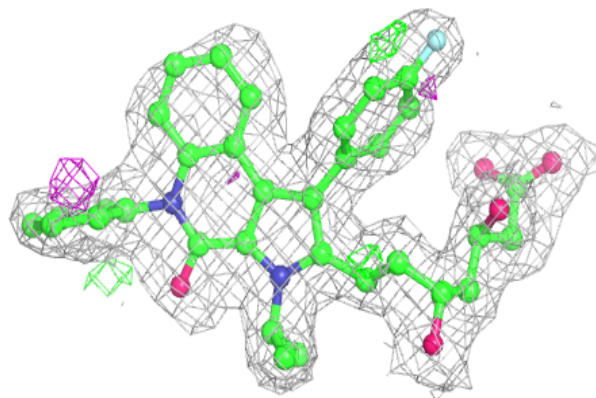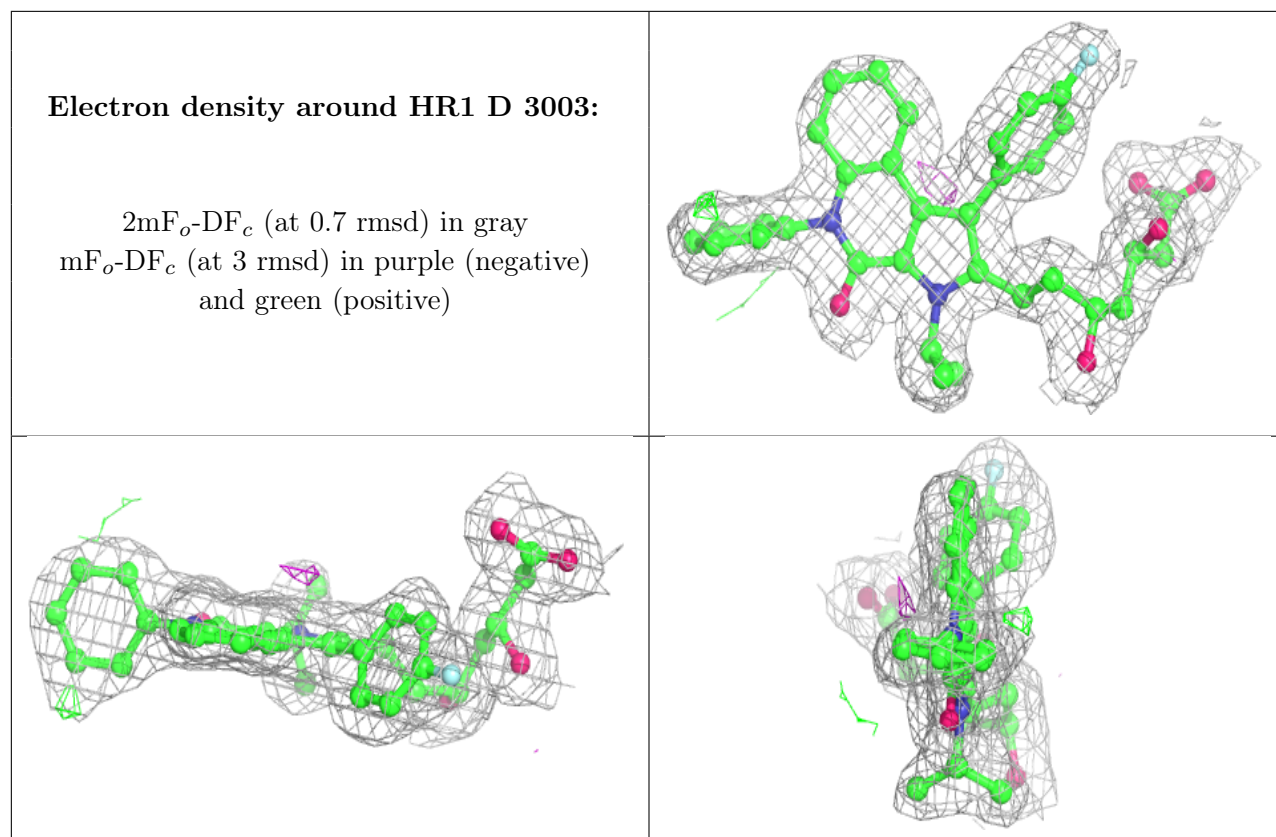
Electron density around HR1 B 3001:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
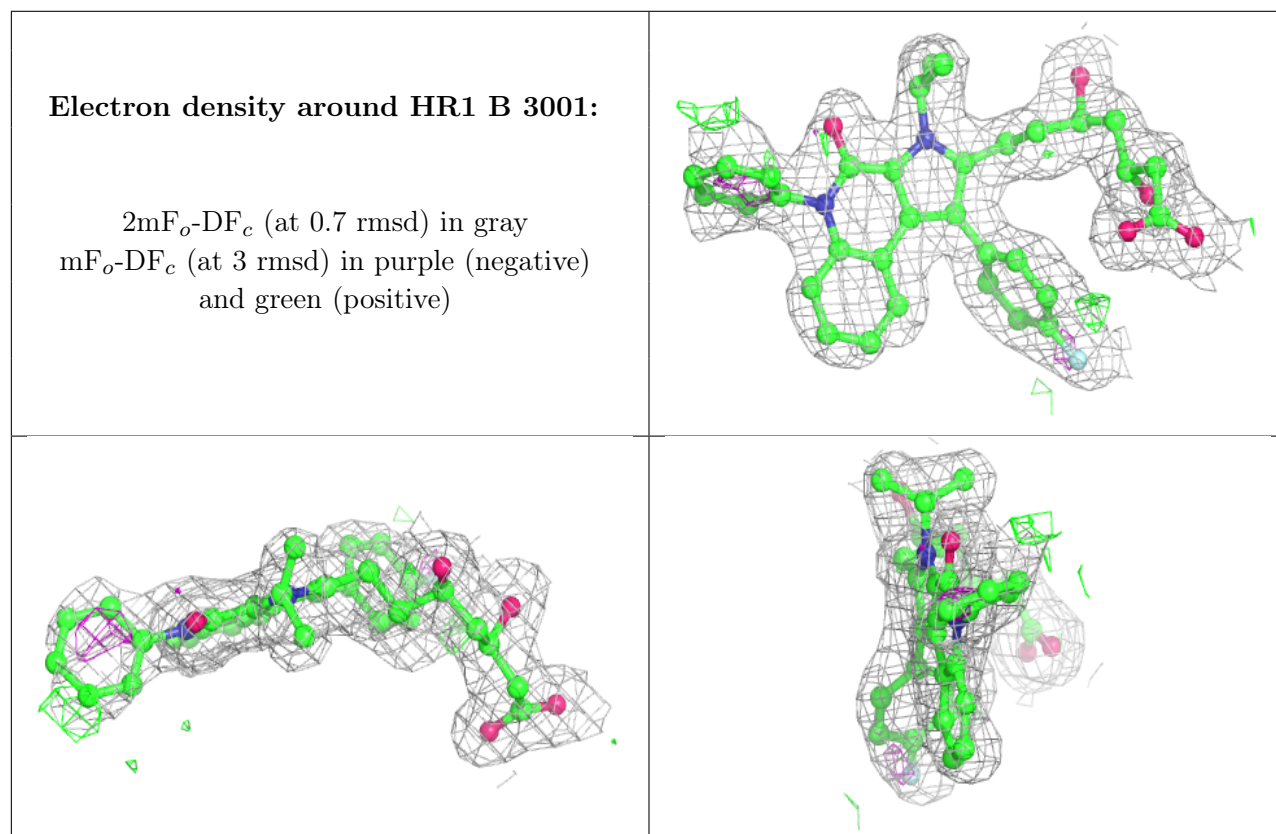
Electron density around HR1 A 3002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
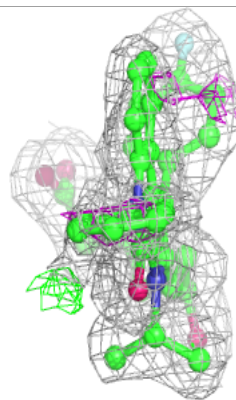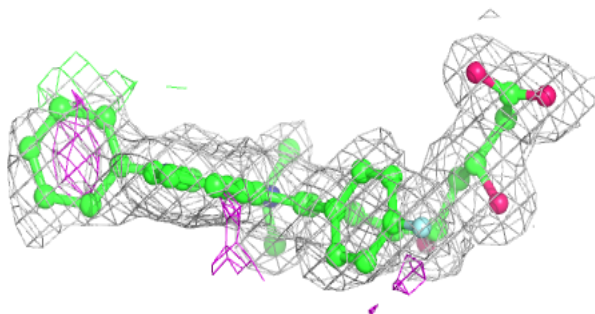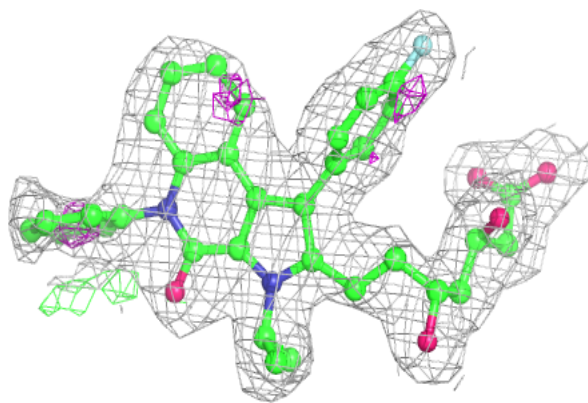
Electron density around HR1 C 3004:

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

Electron density around HR1 D 3003:

$2mF_o$-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 ⓘ

There are no such residues in this entry.