Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2020 – 10:23 AM BST

PDB ID	:	6TPK
Title	:	Crystal structure of the human oxytocin receptor
Authors	:	Waltenspuehl, Y.; Schoeppe, J.; Ehrenmann, J.; Kummer, L.; Plueckthun, A.
Deposited on	:	2019-12-13
Resolution	:	3.20 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:

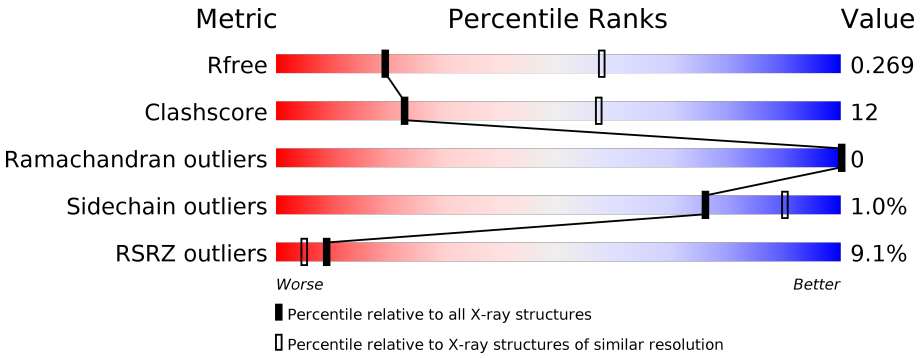
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.6
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.6

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	502	8% 68% 24% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3718 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 Oxytocin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3647	2402	601	615	29			

There are 200 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	HIS	ARG	conflict	UNP P30559
A	120	LEU	VAL	conflict	UNP P30559
A	153	ALA	ASP	conflict	UNP P30559
A	167	VAL	ALA	conflict	UNP P30559
A	193	ARG	GLN	conflict	UNP P30559
A	218	THR	ALA	conflict	UNP P30559
A	224	ALA	SER	conflict	UNP P30559
A	322	CYS	SER	conflict	UNP P30559
A	325	LYS	ASN	conflict	UNP P30559
A	333	MET	THR	conflict	UNP P30559
A	339	GLY	GLU	conflict	UNP P30559
A	340	ILE	LEU	conflict	UNP P30559
A	341	ASP	VAL	conflict	UNP P30559
A	342	YCM	GLN	conflict	UNP P30559
A	343	SER	ARG	conflict	UNP P30559
A	345	TRP	LEU	conflict	UNP P30559
A	348	ASN	SER	conflict	UNP P30559
A	349	GLU	ALA	conflict	UNP P30559
A	353	THR	LYS	conflict	UNP P30559
A	355	SER	ARG	conflict	UNP P30559
A	357	ASP	-	expression tag	UNP P30559
A	358	GLU	-	expression tag	UNP P30559
A	359	ARG	-	expression tag	UNP P30559
A	360	LYS	-	expression tag	UNP P30559
A	361	LYS	-	expression tag	UNP P30559
A	362	SER	-	expression tag	UNP P30559
A	363	LEU	-	expression tag	UNP P30559

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Chain	Residue	Modelled	Actual	Comment	Reference
A	364	LEU	-	expression tag	UNP P30559
A	365	SER	-	expression tag	UNP P30559
A	366	LYS	-	expression tag	UNP P30559
A	367	PHE	-	expression tag	UNP P30559
A	368	GLY	-	expression tag	UNP P30559
A	369	MET	-	expression tag	UNP P30559
A	370	ASP	-	expression tag	UNP P30559
A	371	GLU	-	expression tag	UNP P30559
A	372	GLY	-	expression tag	UNP P30559
A	373	VAL	-	expression tag	UNP P30559
A	374	THR	-	expression tag	UNP P30559
A	375	PHE	-	expression tag	UNP P30559
A	376	MET	-	expression tag	UNP P30559
A	377	PHE	-	expression tag	UNP P30559
A	378	ILE	-	expression tag	UNP P30559
A	379	GLY	-	expression tag	UNP P30559
A	380	ARG	-	expression tag	UNP P30559
A	381	PHE	-	expression tag	UNP P30559
A	382	ASP	-	expression tag	UNP P30559
A	383	ARG	-	expression tag	UNP P30559
A	384	GLY	-	expression tag	UNP P30559
A	385	GLN	-	expression tag	UNP P30559
A	386	LYS	-	expression tag	UNP P30559
A	387	GLY	-	expression tag	UNP P30559
A	388	VAL	-	expression tag	UNP P30559
A	389	ASP	-	expression tag	UNP P30559
A	390	VAL	-	expression tag	UNP P30559
A	391	LEU	-	expression tag	UNP P30559
A	392	LEU	-	expression tag	UNP P30559
A	393	LYS	-	expression tag	UNP P30559
A	394	ALA	-	expression tag	UNP P30559
A	395	ILE	-	expression tag	UNP P30559
A	396	GLU	-	expression tag	UNP P30559
A	397	ILE	-	expression tag	UNP P30559
A	398	LEU	-	expression tag	UNP P30559
A	399	SER	-	expression tag	UNP P30559
A	400	SER	-	expression tag	UNP P30559
A	401	LYS	-	expression tag	UNP P30559
A	402	LYS	-	expression tag	UNP P30559
A	403	GLU	-	expression tag	UNP P30559
A	404	PHE	-	expression tag	UNP P30559
A	405	GLN	-	expression tag	UNP P30559

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Chain	Residue	Modelled	Actual	Comment	Reference
A	406	GLU	-	expression tag	UNP P30559
A	407	MET	-	expression tag	UNP P30559
A	408	ARG	-	expression tag	UNP P30559
A	409	PHE	-	expression tag	UNP P30559
A	410	ILE	-	expression tag	UNP P30559
A	411	ILE	-	expression tag	UNP P30559
A	412	ILE	-	expression tag	UNP P30559
A	413	GLY	-	expression tag	UNP P30559
A	414	LYS	-	expression tag	UNP P30559
A	415	GLY	-	expression tag	UNP P30559
A	416	ASP	-	expression tag	UNP P30559
A	417	PRO	-	expression tag	UNP P30559
A	418	GLU	-	expression tag	UNP P30559
A	419	LEU	-	expression tag	UNP P30559
A	420	GLU	-	expression tag	UNP P30559
A	421	GLY	-	expression tag	UNP P30559
A	422	TRP	-	expression tag	UNP P30559
A	423	ALA	-	expression tag	UNP P30559
A	424	ARG	-	expression tag	UNP P30559
A	425	SER	-	expression tag	UNP P30559
A	426	LEU	-	expression tag	UNP P30559
A	427	GLU	-	expression tag	UNP P30559
A	428	GLU	-	expression tag	UNP P30559
A	429	LYS	-	expression tag	UNP P30559
A	430	HIS	-	expression tag	UNP P30559
A	431	GLY	-	expression tag	UNP P30559
A	432	ASN	-	expression tag	UNP P30559
A	433	VAL	-	expression tag	UNP P30559
A	434	LYS	-	expression tag	UNP P30559
A	435	VAL	-	expression tag	UNP P30559
A	436	ILE	-	expression tag	UNP P30559
A	437	THR	-	expression tag	UNP P30559
A	438	GLU	-	expression tag	UNP P30559
A	439	MET	-	expression tag	UNP P30559
A	440	LEU	-	expression tag	UNP P30559
A	441	SER	-	expression tag	UNP P30559
A	442	ARG	-	expression tag	UNP P30559
A	443	GLU	-	expression tag	UNP P30559
A	444	PHE	-	expression tag	UNP P30559
A	445	VAL	-	expression tag	UNP P30559
A	446	ARG	-	expression tag	UNP P30559
A	447	GLU	-	expression tag	UNP P30559

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Chain	Residue	Modelled	Actual	Comment	Reference
A	448	LEU	-	expression tag	UNP P30559
A	449	TYR	-	expression tag	UNP P30559
A	450	GLY	-	expression tag	UNP P30559
A	451	SER	-	expression tag	UNP P30559
A	452	VAL	-	expression tag	UNP P30559
A	453	ASP	-	expression tag	UNP P30559
A	454	PHE	-	expression tag	UNP P30559
A	455	VAL	-	expression tag	UNP P30559
A	456	ILE	-	expression tag	UNP P30559
A	457	ILE	-	expression tag	UNP P30559
A	458	PRO	-	expression tag	UNP P30559
A	459	SER	-	expression tag	UNP P30559
A	460	TYR	-	expression tag	UNP P30559
A	461	PHE	-	expression tag	UNP P30559
A	462	GLU	-	expression tag	UNP P30559
A	463	PRO	-	expression tag	UNP P30559
A	464	PHE	-	expression tag	UNP P30559
A	465	GLY	-	expression tag	UNP P30559
A	466	LEU	-	expression tag	UNP P30559
A	467	VAL	-	expression tag	UNP P30559
A	468	ALA	-	expression tag	UNP P30559
A	469	LEU	-	expression tag	UNP P30559
A	470	GLU	-	expression tag	UNP P30559
A	471	ALA	-	expression tag	UNP P30559
A	472	MET	-	expression tag	UNP P30559
A	473	CYS	-	expression tag	UNP P30559
A	474	LEU	-	expression tag	UNP P30559
A	475	GLY	-	expression tag	UNP P30559
A	476	ALA	-	expression tag	UNP P30559
A	477	ILE	-	expression tag	UNP P30559
A	478	PRO	-	expression tag	UNP P30559
A	479	ILE	-	expression tag	UNP P30559
A	480	ALA	-	expression tag	UNP P30559
A	481	SER	-	expression tag	UNP P30559
A	482	ALA	-	expression tag	UNP P30559
A	483	VAL	-	expression tag	UNP P30559
A	484	GLY	-	expression tag	UNP P30559
A	485	GLY	-	expression tag	UNP P30559
A	486	LEU	-	expression tag	UNP P30559
A	487	ARG	-	expression tag	UNP P30559
A	488	ASP	-	expression tag	UNP P30559
A	489	ILE	-	expression tag	UNP P30559

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Chain	Residue	Modelled	Actual	Comment	Reference
A	490	ILE	-	expression tag	UNP P30559
A	491	THR	-	expression tag	UNP P30559
A	492	ASN	-	expression tag	UNP P30559
A	493	GLU	-	expression tag	UNP P30559
A	494	THR	-	expression tag	UNP P30559
A	495	GLY	-	expression tag	UNP P30559
A	496	ILE	-	expression tag	UNP P30559
A	497	LEU	-	expression tag	UNP P30559
A	498	VAL	-	expression tag	UNP P30559
A	499	LYS	-	expression tag	UNP P30559
A	500	ALA	-	expression tag	UNP P30559
A	501	GLY	-	expression tag	UNP P30559
A	502	ASP	-	expression tag	UNP P30559
A	503	PRO	-	expression tag	UNP P30559
A	504	GLY	-	expression tag	UNP P30559
A	505	GLU	-	expression tag	UNP P30559
A	506	LEU	-	expression tag	UNP P30559
A	507	ALA	-	expression tag	UNP P30559
A	508	ASN	-	expression tag	UNP P30559
A	509	ALA	-	expression tag	UNP P30559
A	510	ILE	-	expression tag	UNP P30559
A	511	LEU	-	expression tag	UNP P30559
A	512	LYS	-	expression tag	UNP P30559
A	513	ALA	-	expression tag	UNP P30559
A	514	LEU	-	expression tag	UNP P30559
A	515	GLU	-	expression tag	UNP P30559
A	516	LEU	-	expression tag	UNP P30559
A	517	SER	-	expression tag	UNP P30559
A	518	ARG	-	expression tag	UNP P30559
A	519	SER	-	expression tag	UNP P30559
A	520	ASP	-	expression tag	UNP P30559
A	521	LEU	-	expression tag	UNP P30559
A	522	SER	-	expression tag	UNP P30559
A	523	LYS	-	expression tag	UNP P30559
A	524	PHE	-	expression tag	UNP P30559
A	525	ARG	-	expression tag	UNP P30559
A	526	GLU	-	expression tag	UNP P30559
A	527	ASN	-	expression tag	UNP P30559
A	528	CYS	-	expression tag	UNP P30559
A	529	LYS	-	expression tag	UNP P30559
A	530	LYS	-	expression tag	UNP P30559
A	531	ARG	-	expression tag	UNP P30559

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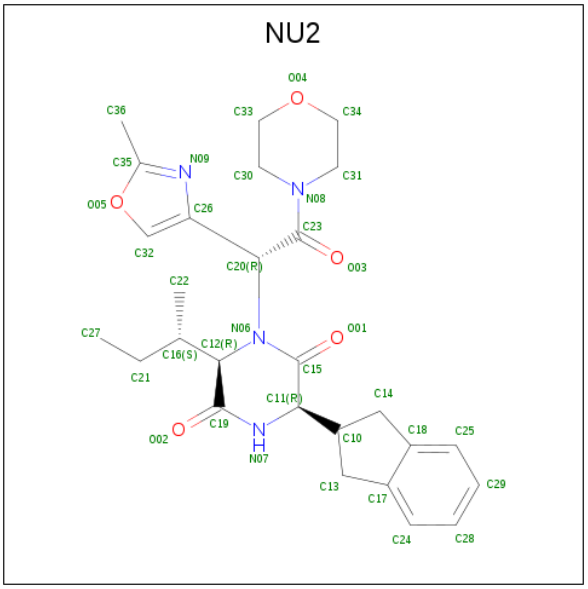
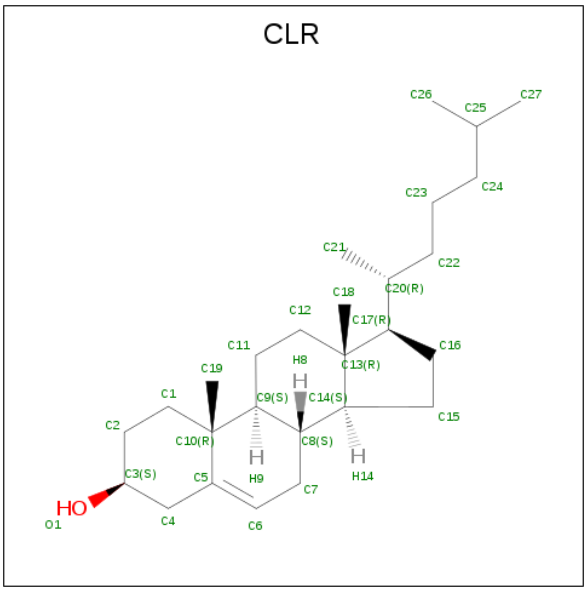
Chain	Residue	Modelled	Actual	Comment	Reference
A	532	ALA	-	expression tag	UNP P30559
A	533	MET	-	expression tag	UNP P30559
A	534	SER	-	expression tag	UNP P30559
A	535	PHE	-	expression tag	UNP P30559
A	536	SER	-	expression tag	UNP P30559

- Molecule 2 is (3 {R},6 {R})-6-[(2 {S})-butan-2-yl]-3-(2,3-dihydro-1 {H}-inden-2-yl)-1-[(1 {R})-1-(2-methyl-1,3-oxazol-4-yl)-2-morpholin-4-yl-2-oxidanylidene-ethyl]piperazine-2,5-dione (three-letter code: NU2) (formula: $C_{27}H_{34}N_4O_5$) (labeled as "Ligand of Interest" by author).



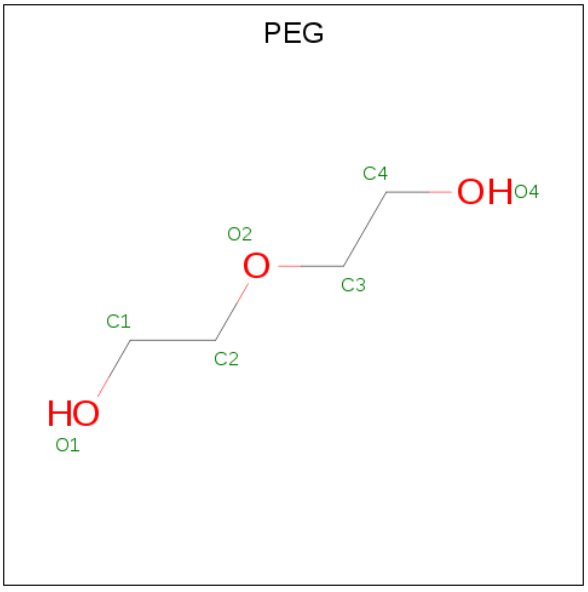
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	27	4	5		

- Molecule 3 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			28	27	1		

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



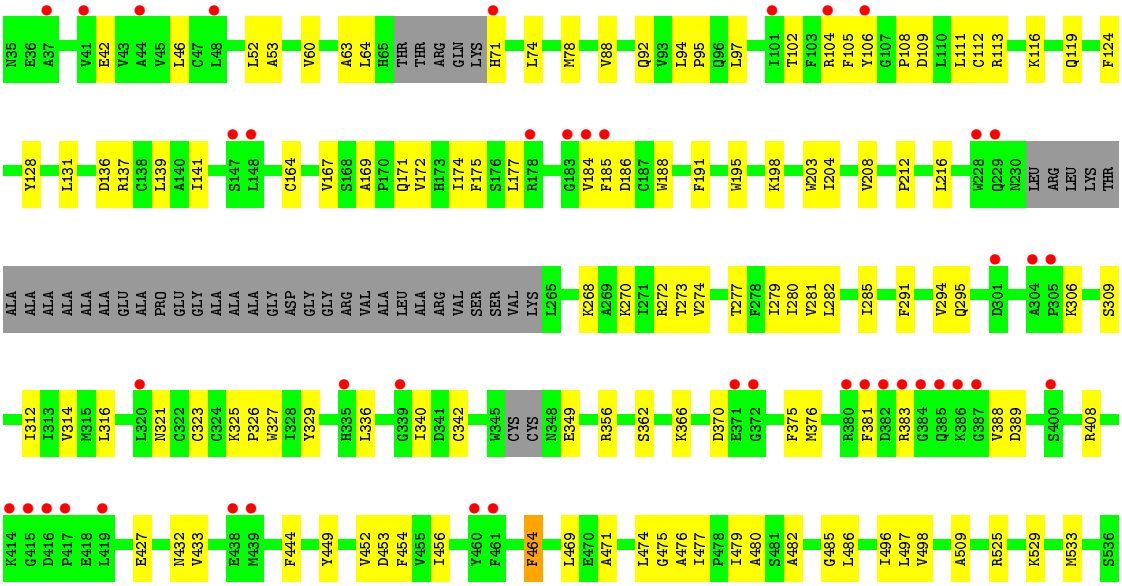
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

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: Oxytocin receptor

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	76.99Å 78.86Å 283.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.84 – 3.20 47.59 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.84-3.20) 99.7 (47.59-3.20)	Depositor EDS
R_{merge}	0.49	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.252 , 0.266 0.257 , 0.269	Depositor DCC
R_{free} test set	632 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å^2)	88.6	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.059 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3718	wwPDB-VP
Average B, all atoms (Å^2)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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, NU2, YCM, CLR

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	0/3718	0.50	0/5031

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	3647	0	3770	87	0
2	A	36	0	0	1	0
3	A	28	0	46	0	0
4	A	7	0	10	0	0
All	All	3718	0	3826	87	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 (87) 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:52:LEU:HD13	1:A:327:TRP:CZ2	2.07	0.89
1:A:52:LEU:CD1	1:A:327:TRP:HZ2	1.88	0.86
1:A:52:LEU:HD13	1:A:327:TRP:HZ2	1.41	0.82
1:A:52:LEU:HD12	1:A:323:CYS:HB2	1.61	0.80
1:A:277:THR:HA	1:A:280:ILE:HD12	1.67	0.76
1:A:105:PHE:HB2	1:A:186:ASP:HA	1.71	0.73
1:A:71:HIS:HB3	1:A:137:ARG:HH22	1.53	0.72
1:A:52:LEU:CD1	1:A:327:TRP:CZ2	2.71	0.72
1:A:52:LEU:CD1	1:A:323:CYS:HB2	2.19	0.72
1:A:174:ILE:HG23	1:A:175:PHE:HD1	1.55	0.70
1:A:174:ILE:HD11	1:A:191:PHE:CE1	2.28	0.68
1:A:306:LYS:HG2	1:A:309:SER:HB2	1.75	0.68
1:A:480:ALA:HB1	1:A:486:LEU:HD13	1.78	0.64
1:A:342:YCM:HD3	1:A:533:MET:HG2	1.78	0.64
1:A:498:VAL:HG11	1:A:509:ALA:HB2	1.80	0.62
1:A:356:ARG:NH2	1:A:449:TYR:O	2.33	0.62
1:A:53:ALA:HB2	1:A:323:CYS:HB3	1.83	0.60
1:A:92:GLN:OE1	1:A:119:GLN:NE2	2.35	0.60
1:A:137:ARG:HB3	1:A:274:VAL:HG22	1.84	0.60
1:A:171:GLN:HA	1:A:174:ILE:HG22	1.83	0.59
1:A:74:LEU:HD22	1:A:273:THR:HB	1.84	0.58
1:A:375:PHE:HB3	1:A:456:ILE:HD11	1.86	0.58
1:A:312:ILE:O	1:A:316:LEU:HG	2.04	0.58
1:A:376:MET:HB2	1:A:452:VAL:HG11	1.84	0.57
1:A:370:ASP:HB2	1:A:408:ARG:HH21	1.69	0.57
1:A:88:VAL:O	1:A:92:GLN:HB3	2.04	0.56
1:A:362:SER:O	1:A:366:LYS:HG2	2.05	0.56
1:A:321:ASN:OD1	1:A:325:LYS:NZ	2.38	0.56
1:A:169:ALA:O	1:A:172:VAL:HG12	2.06	0.56
1:A:104:ARG:HG2	1:A:184:VAL:HG13	1.87	0.56
1:A:216:LEU:HD13	1:A:281:VAL:HG13	1.88	0.55
1:A:167:VAL:HG13	1:A:203:TRP:HZ2	1.72	0.54
1:A:52:LEU:HD11	1:A:323:CYS:SG	2.47	0.54
1:A:204:ILE:O	1:A:208:VAL:HG22	2.07	0.53
1:A:356:ARG:HH11	1:A:525:ARG:HD3	1.72	0.53
1:A:128:TYR:HE1	1:A:212:PRO:HG3	1.74	0.53
1:A:471:ALA:HB1	1:A:476:ALA:HB3	1.91	0.52
1:A:94:LEU:HB3	1:A:95:PRO:HD3	1.91	0.52
1:A:74:LEU:CD2	1:A:273:THR:HB	2.39	0.52
1:A:71:HIS:CE1	1:A:136:ASP:OD1	2.63	0.52
1:A:109:ASP:O	1:A:112:CYS:HB3	2.09	0.52
1:A:71:HIS:ND1	1:A:136:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:TRP:O	1:A:198:LYS:HG2	2.11	0.51
1:A:349:GLU:HB2	1:A:529:LYS:HZ2	1.76	0.51
1:A:171:GLN:NE2	2:A:1501:NU2:O02	2.44	0.50
1:A:268:LYS:O	1:A:272:ARG:HG2	2.11	0.50
1:A:381:PHE:CE1	1:A:388:VAL:HG21	2.46	0.50
1:A:46:LEU:HB3	1:A:97:LEU:HD13	1.92	0.50
1:A:42:GLU:HG2	1:A:316:LEU:HD21	1.94	0.49
1:A:60:VAL:O	1:A:64:LEU:HG	2.13	0.49
1:A:105:PHE:CB	1:A:186:ASP:HA	2.41	0.48
1:A:177:LEU:HD22	1:A:185:PHE:HB3	1.95	0.48
1:A:113:ARG:HB3	1:A:172:VAL:HG23	1.94	0.48
1:A:136:ASP:O	1:A:139:LEU:HG	2.14	0.48
1:A:116:LYS:HE2	1:A:175:PHE:CE2	2.49	0.47
1:A:356:ARG:HH12	1:A:475:GLY:C	2.16	0.47
1:A:108:PRO:HD2	1:A:111:LEU:HD13	1.95	0.47
1:A:340:ILE:HD12	1:A:469:LEU:HB3	1.97	0.47
1:A:306:LYS:HE3	1:A:309:SER:HB2	1.96	0.47
1:A:63:ALA:HB1	1:A:336:LEU:HG	1.97	0.46
1:A:282:LEU:O	1:A:285:ILE:HG13	2.17	0.45
1:A:71:HIS:CD2	1:A:71:HIS:O	2.69	0.45
1:A:323:CYS:O	1:A:326:PRO:HD2	2.16	0.45
1:A:464:PHE:HA	1:A:485:GLY:HA3	1.99	0.45
1:A:102:THR:HG1	1:A:106:TYR:HE2	1.65	0.45
1:A:124:PHE:HB3	1:A:164:CYS:SG	2.57	0.44
1:A:52:LEU:CD2	1:A:327:TRP:HZ2	2.31	0.44
1:A:141:ILE:HD13	1:A:270:LYS:HE3	2.00	0.44
1:A:52:LEU:HD13	1:A:327:TRP:CE2	2.48	0.44
1:A:128:TYR:CD1	1:A:131:LEU:HD12	2.54	0.43
1:A:381:PHE:HD1	1:A:388:VAL:HG11	1.84	0.43
1:A:482:ALA:HA	1:A:497:LEU:HD22	1.99	0.43
1:A:453:ASP:HA	1:A:525:ARG:HH21	1.83	0.43
1:A:92:GLN:HA	1:A:119:GLN:HE21	1.82	0.43
1:A:131:LEU:HD11	1:A:212:PRO:HA	1.99	0.43
1:A:449:TYR:HB3	1:A:474:LEU:HB2	2.00	0.43
1:A:383:ARG:HD3	1:A:389:ASP:OD2	2.18	0.43
1:A:408:ARG:HD3	1:A:432:ASN:HB2	2.01	0.42
1:A:78:MET:HG2	1:A:329:TYR:CZ	2.54	0.42
1:A:479:ILE:HG23	1:A:496:ILE:HB	2.01	0.42
1:A:427:GLU:HG3	1:A:433:VAL:O	2.19	0.42
1:A:454:PHE:CD1	1:A:477:ILE:HB	2.55	0.42
1:A:294:VAL:HG21	1:A:314:VAL:HG11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:NH1	1:A:525:ARG:HD3	2.35	0.41
1:A:279:ILE:HA	1:A:279:ILE:HD13	1.94	0.41
1:A:291:PHE:HA	1:A:314:VAL:HB	2.01	0.41
1:A:381:PHE:CD1	1:A:388:VAL:HG21	2.56	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	452/502 (90%)	434 (96%)	18 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	391/419 (93%)	387 (99%)	4 (1%)	76 90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	TRP
1	A	295	GLN

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Mol	Chain	Res	Type
1	A	444	PHE
1	A	464	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	YCM	A	342	1	7,9,10	0.47	0	4,10,12	0.43	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
1	YCM	A	342	1	-	1/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	342	YCM	CA-CB-SG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	342	YCM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	CLR	A	1502	-	31,31,31	0.31	0	48,48,48	0.78	2 (4%)
2	NU2	A	1501	-	34,40,40	4.72	16 (47%)	42,58,58	2.22	12 (28%)
4	PEG	A	1503	-	6,6,6	0.44	0	5,5,5	0.28	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	CLR	A	1502	-	-	6/10/68/68	0/4/4/4
2	NU2	A	1501	-	-	6/22/62/62	0/5/5/5
4	PEG	A	1503	-	-	1/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1501	NU2	C23-N08	10.15	1.49	1.34
2	A	1501	NU2	C25-C18	9.84	1.56	1.39
2	A	1501	NU2	C24-C17	9.75	1.56	1.39
2	A	1501	NU2	C19-N07	9.51	1.48	1.33
2	A	1501	NU2	C28-C24	7.96	1.55	1.38
2	A	1501	NU2	C29-C25	7.77	1.55	1.38
2	A	1501	NU2	C15-N06	7.75	1.47	1.35
2	A	1501	NU2	C29-C28	5.95	1.53	1.38
2	A	1501	NU2	C18-C17	5.90	1.50	1.39
2	A	1501	NU2	C36-C35	5.68	1.55	1.49
2	A	1501	NU2	C26-C20	-4.40	1.50	1.53
2	A	1501	NU2	C13-C17	3.94	1.57	1.50
2	A	1501	NU2	C20-C23	3.34	1.57	1.54
2	A	1501	NU2	C13-C10	-2.69	1.49	1.54
2	A	1501	NU2	C12-N06	2.43	1.51	1.47
2	A	1501	NU2	C12-C19	2.13	1.54	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1501	NU2	C13-C17-C18	-5.87	106.53	110.56
2	A	1501	NU2	C14-C18-C17	-5.43	106.83	110.56
2	A	1501	NU2	C20-C23-N08	4.94	122.20	117.38
2	A	1501	NU2	C26-C20-N06	3.70	116.76	111.25
2	A	1501	NU2	O03-C23-N08	-3.23	117.88	121.67
2	A	1501	NU2	C20-N06-C12	3.15	125.83	118.67
2	A	1501	NU2	C17-C13-C10	-3.04	99.76	104.06
2	A	1501	NU2	C12-N06-C15	-3.02	115.88	122.53
3	A	1502	CLR	C16-C17-C13	-2.70	100.59	103.84
2	A	1501	NU2	O02-C19-N07	-2.58	119.22	122.69
2	A	1501	NU2	C11-N07-C19	-2.57	118.12	124.63
2	A	1501	NU2	C13-C17-C24	2.29	133.46	129.18
3	A	1502	CLR	C15-C14-C13	2.16	106.44	103.84
2	A	1501	NU2	C22-C16-C21	-2.02	106.66	111.78

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	NU2	C13-C10-C11-C15
2	A	1501	NU2	C13-C10-C11-N07
2	A	1501	NU2	C14-C10-C11-N07

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Mol	Chain	Res	Type	Atoms
2	A	1501	NU2	C26-C20-N06-C15
2	A	1501	NU2	C26-C20-N06-C12
4	A	1503	PEG	O2-C3-C4-O4
3	A	1502	CLR	C16-C17-C20-C22
3	A	1502	CLR	C20-C22-C23-C24
3	A	1502	CLR	C22-C23-C24-C25
3	A	1502	CLR	C13-C17-C20-C21
3	A	1502	CLR	C16-C17-C20-C21
3	A	1502	CLR	C21-C20-C22-C23
2	A	1501	NU2	N06-C20-C23-O03

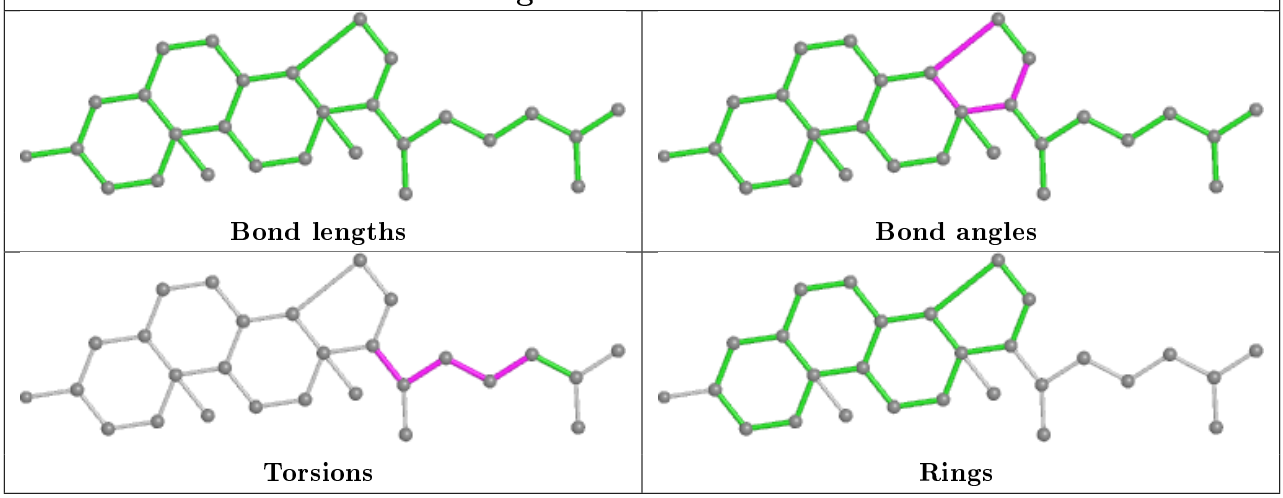
There are no ring outliers.

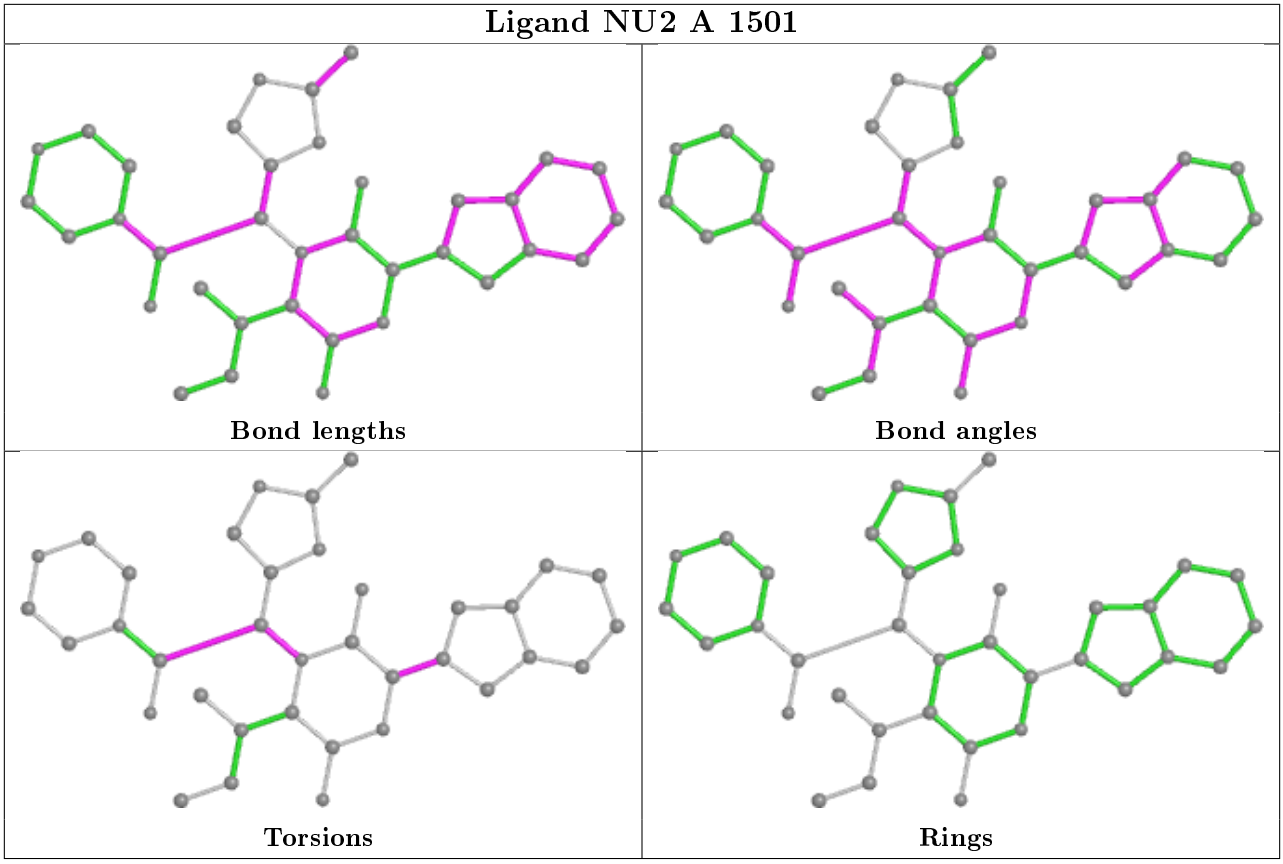
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	NU2	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 CLR A 1502





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	338:HIS	C	339:GLY	N	35.58
1	A	265:LEU	C	266:ILE	N	7.89

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	460/502 (91%)	0.27	42 (9%) 9 5	48, 96, 164, 224	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	HIS	7.1
1	A	415	GLY	6.2
1	A	416	ASP	6.1
1	A	382	ASP	5.7
1	A	384	GLY	5.6
1	A	106	TYR	5.6
1	A	229	GLN	5.4
1	A	414	LYS	5.3
1	A	183	GLY	4.9
1	A	228	TRP	4.8
1	A	438	GLU	4.7
1	A	104	ARG	4.6
1	A	385	GLN	4.4
1	A	380	ARG	4.3
1	A	101	ILE	4.1
1	A	301	ASP	3.9
1	A	383	ARG	3.8
1	A	419	LEU	3.6
1	A	148	LEU	3.6
1	A	381	PHE	3.5
1	A	339	GLY	3.3
1	A	147	SER	3.3
1	A	386	LYS	3.3
1	A	185	PHE	3.2
1	A	178	ARG	3.1
1	A	417	PRO	3.1
1	A	184	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	400	SER	2.6
1	A	320	LEU	2.3
1	A	305	PRO	2.3
1	A	48	LEU	2.3
1	A	37	ALA	2.3
1	A	439	MET	2.3
1	A	461	PHE	2.2
1	A	335	HIS	2.2
1	A	44	ALA	2.1
1	A	41	VAL	2.1
1	A	372	GLY	2.1
1	A	304	ALA	2.0
1	A	460	TYR	2.0
1	A	387	GLY	2.0
1	A	371	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	YCM	A	342	10/11	0.89	0.18	79,88,94,97	0

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
4	PEG	A	1503	7/7	0.76	0.26	59,76,92,93	0
2	NU2	A	1501	36/36	0.88	0.25	90,113,155,161	0

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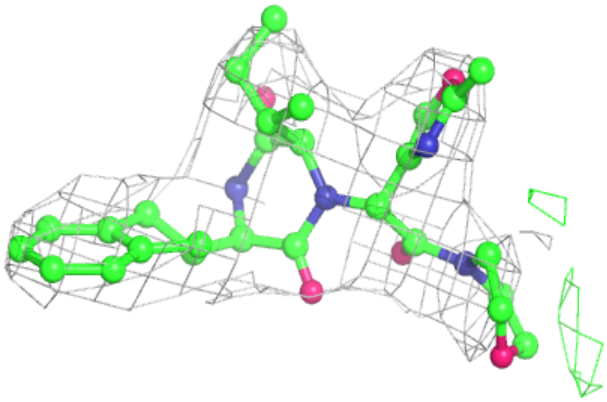
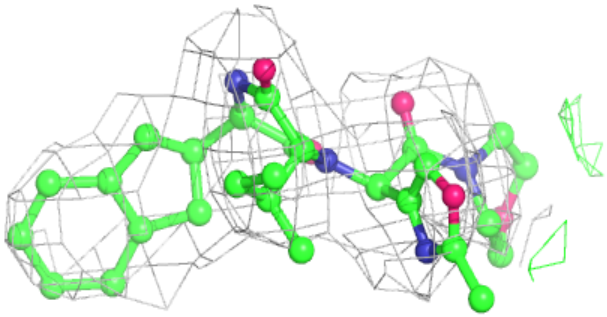
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CLR	A	1502	28/28	0.89	0.40	98,113,118,120	0

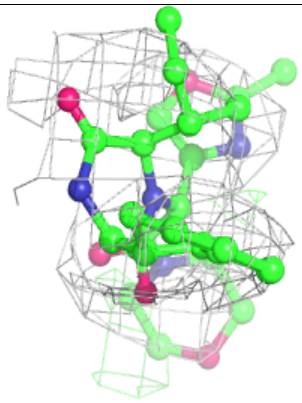
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NU2 A 1501:

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

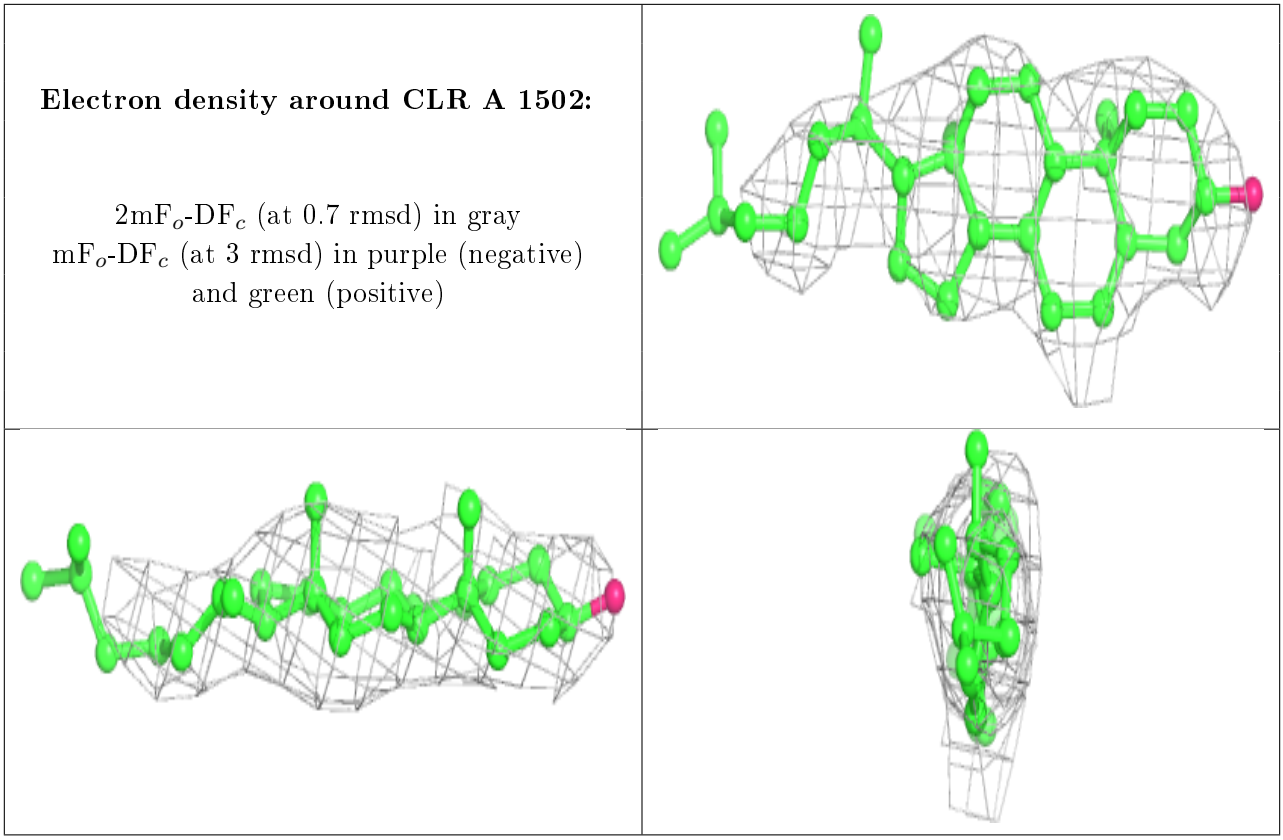






Electron density around CLR A 1502:

$2mF_o$-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.