Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 12:30 PM EDT

PDB ID	:	3H52
Title	:	Crystal structure of the antagonist form of human glucocorticoid receptor
Authors	:	Schoch, G.A.; Benz, J.; D'Arcy, B.; Stihle, M.; Burger, D.; Thoma, R.; Ruf, A.
Deposited on	:	2009-04-21
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

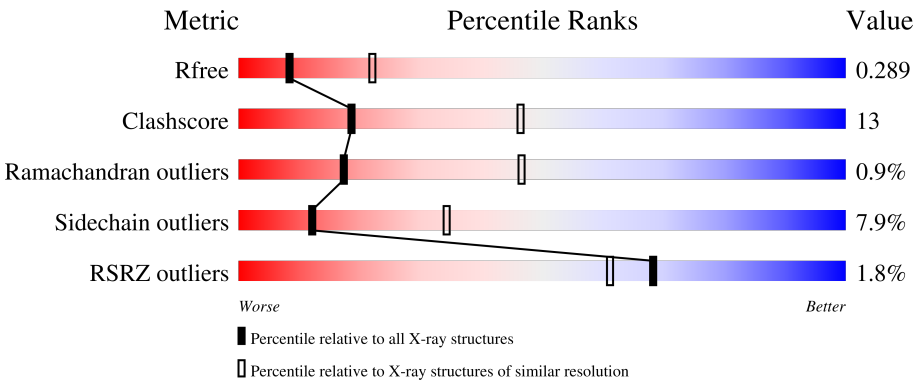
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	254	70% 24%
1	B	254	72% 21%
1	C	254	66% 26% 7%
1	D	254	65% 25% 8%
2	M	19	26% 26% 47%

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Mol	Chain	Length	Quality of chain
2	N	19	5% 63% 11% 5% 21%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7989 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 Glucocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	247	1964	1265	325	357	17	0	0	0
1	B	249	1986	1279	327	363	17	0	0	0
1	C	237	1845	1180	314	336	15	0	0	0
1	D	234	1855	1193	308	338	16	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	524	GLY	-	expression tag	UNP P04150
A	525	SER	-	expression tag	UNP P04150
A	526	HIS	-	expression tag	UNP P04150
A	527	MET	-	expression tag	UNP P04150
A	602	SER	PHE	engineered mutation	UNP P04150
A	638	ASP	CYS	engineered mutation	UNP P04150
A	684	ALA	GLU	engineered mutation	UNP P04150
A	688	ALA	GLU	engineered mutation	UNP P04150
A	712	SER	TRP	engineered mutation	UNP P04150
B	524	GLY	-	expression tag	UNP P04150
B	525	SER	-	expression tag	UNP P04150
B	526	HIS	-	expression tag	UNP P04150
B	527	MET	-	expression tag	UNP P04150
B	602	SER	PHE	engineered mutation	UNP P04150
B	638	ASP	CYS	engineered mutation	UNP P04150
B	684	ALA	GLU	engineered mutation	UNP P04150
B	688	ALA	GLU	engineered mutation	UNP P04150
B	712	SER	TRP	engineered mutation	UNP P04150
C	524	GLY	-	expression tag	UNP P04150
C	525	SER	-	expression tag	UNP P04150
C	526	HIS	-	expression tag	UNP P04150

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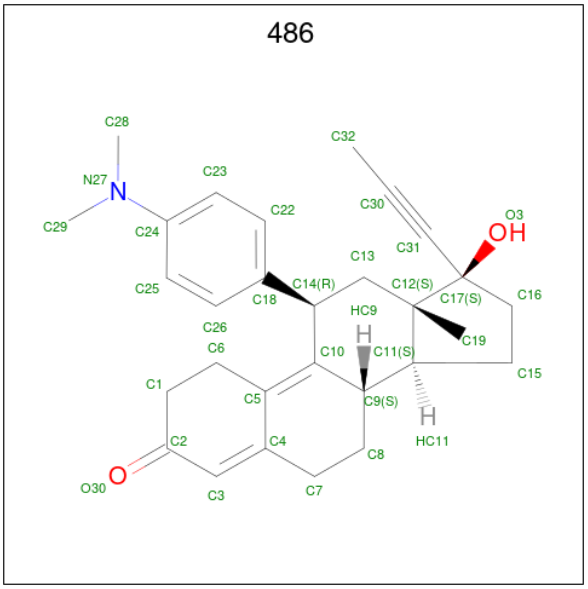
Chain	Residue	Modelled	Actual	Comment	Reference
C	527	MET	-	expression tag	UNP P04150
C	602	SER	PHE	engineered mutation	UNP P04150
C	638	ASP	CYS	engineered mutation	UNP P04150
C	684	ALA	GLU	engineered mutation	UNP P04150
C	688	ALA	GLU	engineered mutation	UNP P04150
C	712	SER	TRP	engineered mutation	UNP P04150
D	524	GLY	-	expression tag	UNP P04150
D	525	SER	-	expression tag	UNP P04150
D	526	HIS	-	expression tag	UNP P04150
D	527	MET	-	expression tag	UNP P04150
D	602	SER	PHE	engineered mutation	UNP P04150
D	638	ASP	CYS	engineered mutation	UNP P04150
D	684	ALA	GLU	engineered mutation	UNP P04150
D	688	ALA	GLU	engineered mutation	UNP P04150
D	712	SER	TRP	engineered mutation	UNP P04150

- Molecule 2 is a protein called Nuclear receptor corepressor 1.

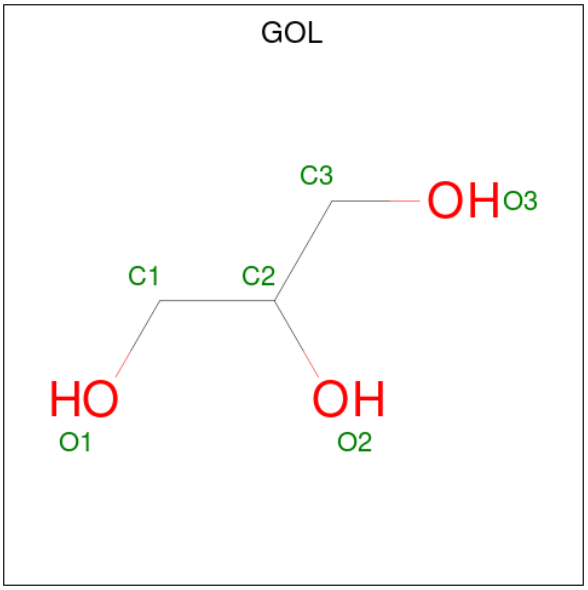
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	15	106	66	19	20	1	0	0	0
			Total	C	N	O	S			
2	M	10	72	44	14	13	1	0	0	0

- Molecule 3 is 11-(4-DIMETHYLAMINO-PHENYL)-17-HYDROXY-13-METHYL-17-PROP-1-YNYL-1,2,6,7,8,11,12,13,14,15,16,17-DODEC AHYDRO-CYCLOPENTA[A]PHENANTHREN-3-ONE (three-letter code: 486) (formula: $C_{29}H_{35}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	32	29	1	2	0	0
3	B	1	32	29	1	2	0	0
3	C	1	32	29	1	2	0	0
3	D	1	32	29	1	2	0	0

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	8	8	8	0	0
5	B	4	4	4	0	0
5	C	1	1	1	0	0
5	D	11	11	11	0	0
5	N	2	2	2	0	0

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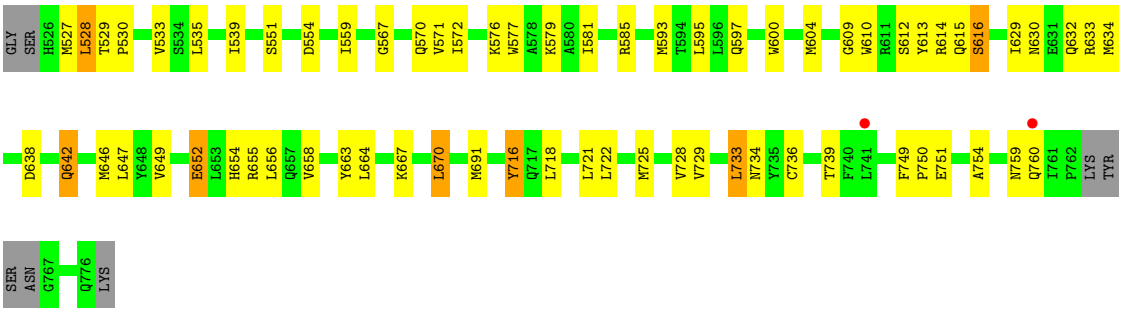
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	M	1	1	1	0	0

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.

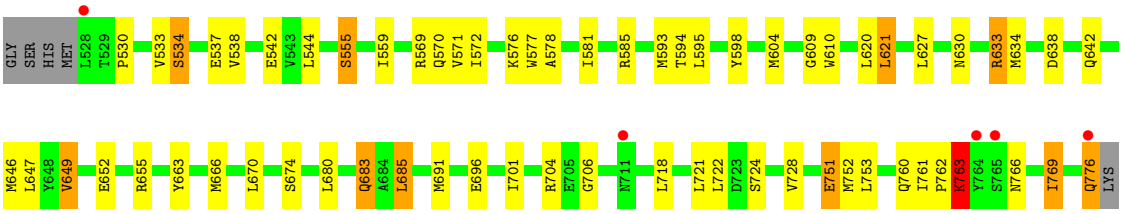
• Molecule 1: Glucocorticoid receptor

Chain A:



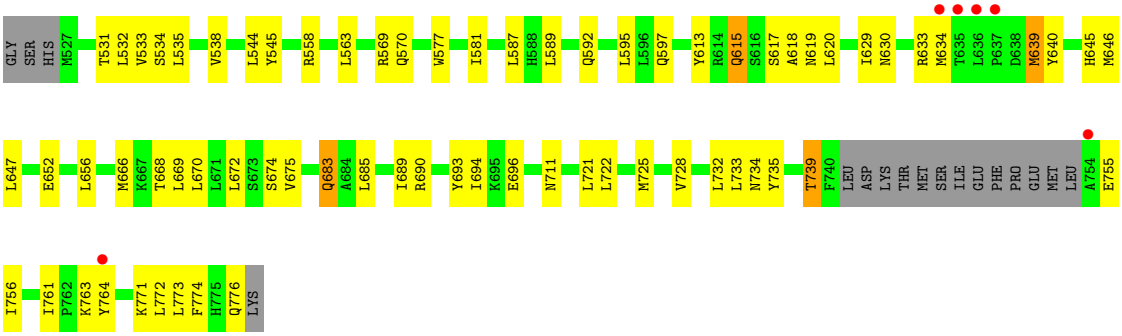
• Molecule 1: Glucocorticoid receptor

Chain B:



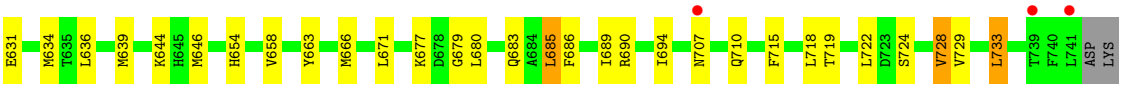
• Molecule 1: Glucocorticoid receptor

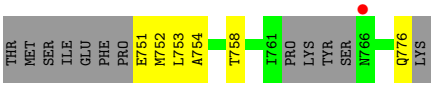
Chain C:



• Molecule 1: Glucocorticoid receptor

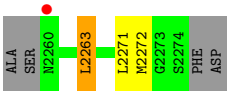
Chain D:





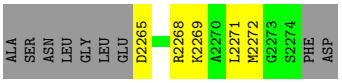
• Molecule 2: Nuclear receptor corepressor 1

Chain N:



• Molecule 2: Nuclear receptor corepressor 1

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.53Å 99.53Å 252.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.10 – 2.80 43.10 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (43.10-2.80) 99.8 (43.10-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.226 , 0.283 0.232 , 0.289	Depositor DCC
R_{free} test set	1830 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	66.3	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7989	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 486, GOL

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	0.46	0/2004	0.58	0/2711
1	B	0.45	0/2028	0.58	0/2746
1	C	0.41	0/1880	0.56	0/2547
1	D	0.43	0/1891	0.58	0/2556
2	M	0.55	0/71	0.63	0/92
2	N	0.49	0/105	0.68	0/138
All	All	0.44	0/7979	0.58	0/10790

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	616	SER	Peptide

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	1964	0	1965	53	0
1	B	1986	0	1987	60	0
1	C	1845	0	1816	47	0
1	D	1855	0	1848	54	0
2	M	72	0	75	3	0
2	N	106	0	108	7	0
3	A	32	0	35	5	0
3	B	32	0	35	9	0
3	C	32	0	35	7	0
3	D	32	0	35	14	0
4	B	6	0	8	0	0
5	A	8	0	0	0	0
5	B	4	0	0	0	0
5	C	1	0	0	0	0
5	D	11	0	0	1	0
5	M	1	0	0	1	0
5	N	2	0	0	0	0
All	All	7989	0	7947	210	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 13.

All (210) 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:D:685:LEU:HD13	1:D:689:ILE:HD11	1.41	1.02
1:A:652:GLU:HG2	1:A:721:LEU:HD13	1.46	0.98
1:A:571:VAL:HG22	1:A:604:MET:HE1	1.46	0.95
1:A:634:MET:HE1	1:A:647:LEU:HD11	1.50	0.93
1:A:670:LEU:HD13	1:A:722:LEU:HD22	1.48	0.93
1:C:570:GLN:HE22	3:C:4:486:C2	1.87	0.88
1:D:639:MET:CE	3:D:2:486:C32	2.51	0.87
1:B:571:VAL:HG22	1:B:604:MET:HE1	1.57	0.84
1:B:534:SER:O	1:B:538:VAL:HG23	1.78	0.83
1:D:639:MET:CE	3:D:2:486:H322	2.10	0.81
1:B:701:ILE:HD11	1:B:718:LEU:HD12	1.65	0.78
1:D:595:LEU:HD11	1:D:680:LEU:HD11	1.67	0.77
1:D:685:LEU:CD1	1:D:689:ILE:HD11	2.14	0.77
1:D:570:GLN:HE22	3:D:2:486:C2	1.98	0.76
1:A:571:VAL:HG22	1:A:604:MET:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:MET:O	1:A:649:VAL:HG12	1.83	0.76
1:D:685:LEU:HD13	1:D:689:ILE:CD1	2.15	0.76
1:B:577:TRP:CZ2	1:B:581:ILE:HD11	2.21	0.75
1:A:759:ASN:CB	2:N:2263:LEU:HD13	2.17	0.74
1:A:559:ILE:HD11	1:A:629:ILE:HD11	1.69	0.74
1:A:581:ILE:O	1:A:585:ARG:HG2	1.87	0.73
1:D:753:LEU:CB	3:D:2:486:H293	2.19	0.73
3:D:2:486:C18	3:D:2:486:H192	2.18	0.72
1:B:571:VAL:HG21	3:B:1:486:H283	1.72	0.71
1:A:577:TRP:CZ2	1:A:581:ILE:HD11	2.25	0.71
1:B:642:GLN:OE1	3:B:1:486:C30	2.38	0.71
1:A:634:MET:CE	1:A:647:LEU:HD11	2.22	0.70
1:D:639:MET:HE1	3:D:2:486:H323	1.73	0.70
1:C:725:MET:HA	1:C:728:VAL:HG12	1.74	0.69
2:M:2265:ASP:N	5:M:8:HOH:O	2.23	0.69
1:C:620:LEU:HD22	1:C:630:ASN:HA	1.75	0.69
1:D:639:MET:HE1	3:D:2:486:C32	2.22	0.68
1:D:639:MET:CE	3:D:2:486:H323	2.23	0.67
1:A:615:GLN:O	1:A:615:GLN:HG3	1.94	0.67
1:D:690:ARG:NH1	1:D:694:ILE:HD11	2.11	0.66
1:D:601:MET:HG2	1:D:733:LEU:HD13	1.77	0.65
1:D:686:PHE:HA	1:D:689:ILE:HD12	1.79	0.65
1:B:578:ALA:HA	1:B:581:ILE:HD12	1.79	0.64
1:B:533:VAL:HG23	1:C:696:GLU:OE2	1.99	0.63
1:C:534:SER:O	1:C:538:VAL:HG23	1.99	0.62
1:D:729:VAL:HG13	1:D:733:LEU:HD22	1.81	0.62
1:C:652:GLU:HG2	1:C:721:LEU:HD13	1.82	0.61
1:B:670:LEU:HD11	1:B:722:LEU:HD22	1.82	0.61
1:A:634:MET:HE1	1:A:647:LEU:CD1	2.28	0.61
1:B:646:MET:HE1	3:B:1:486:H322	1.83	0.61
1:B:577:TRP:CE2	1:B:581:ILE:HD11	2.37	0.60
1:A:670:LEU:CD1	1:A:722:LEU:HD22	2.29	0.60
1:B:620:LEU:HD22	1:B:630:ASN:HA	1.82	0.60
1:B:594:THR:HG22	1:B:598:TYR:CE2	2.37	0.60
1:A:610:TRP:CZ2	1:A:614:ARG:HD2	2.37	0.60
1:B:544:LEU:HD21	1:C:569:ARG:HB3	1.83	0.59
1:A:559:ILE:HD11	1:A:629:ILE:CD1	2.32	0.59
1:B:570:GLN:HE21	1:B:604:MET:HG2	1.68	0.59
1:A:528:LEU:HD12	1:A:529:THR:H	1.69	0.58
1:B:652:GLU:HG2	1:B:721:LEU:HD13	1.84	0.58
1:C:589:LEU:HD23	1:C:592:GLN:NE2	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:670:LEU:CD1	1:B:722:LEU:HD22	2.33	0.57
1:C:771:LYS:O	1:C:773:LEU:HD23	2.04	0.57
1:B:776:GLN:HE21	1:B:776:GLN:C	2.08	0.57
1:A:600:TRP:CZ2	2:N:2263:LEU:HD11	2.39	0.57
1:D:620:LEU:HD22	1:D:630:ASN:HA	1.85	0.57
1:D:534:SER:O	1:D:538:VAL:HG23	2.05	0.57
1:B:569:ARG:NH2	1:C:545:TYR:O	2.36	0.56
1:A:570:GLN:HE22	3:A:3:486:C2	2.18	0.56
1:A:577:TRP:CE2	1:A:581:ILE:HD11	2.40	0.56
1:D:666:MET:HB3	1:D:722:LEU:HD21	1.88	0.56
1:A:600:TRP:CE2	2:N:2263:LEU:HD11	2.40	0.56
1:C:629:ILE:HG22	1:C:634:MET:HG3	1.88	0.56
1:C:645:HIS:HB3	1:C:728:VAL:HG23	1.88	0.55
1:D:724:SER:O	1:D:728:VAL:HG13	2.06	0.55
3:D:2:486:C18	3:D:2:486:C19	2.84	0.54
1:D:559:ILE:HD12	1:D:629:ILE:HD11	1.89	0.54
3:A:3:486:C5	3:A:3:486:HC26	2.36	0.54
1:B:642:GLN:OE1	3:B:1:486:H323	2.07	0.54
1:D:715:PHE:O	1:D:719:THR:OG1	2.18	0.54
1:B:530:PRO:HB3	1:B:534:SER:HB2	1.90	0.53
1:B:559:ILE:HD12	1:B:633:ARG:NH2	2.24	0.53
1:B:683:GLN:HA	1:B:683:GLN:HE21	1.73	0.53
1:B:769:ILE:HG23	1:B:769:ILE:O	2.09	0.53
1:C:615:GLN:HG3	1:D:538:VAL:HG13	1.90	0.53
1:D:658:VAL:HG22	1:D:718:LEU:HD21	1.91	0.53
1:D:577:TRP:CZ2	1:D:581:ILE:HD11	2.44	0.53
1:D:639:MET:HE2	3:D:2:486:H322	1.90	0.52
1:A:571:VAL:HA	1:A:604:MET:HE2	1.91	0.52
1:C:629:ILE:HG23	1:C:633:ARG:HB3	1.92	0.52
1:C:735:TYR:O	1:C:739:THR:N	2.41	0.52
1:D:639:MET:HE3	3:D:2:486:H322	1.89	0.52
1:A:539:ILE:HD11	1:D:581:ILE:HD13	1.91	0.52
1:B:577:TRP:CH2	1:B:581:ILE:HD11	2.44	0.52
1:B:680:LEU:HB2	1:B:683:GLN:HG2	1.92	0.51
1:D:595:LEU:HD13	1:D:680:LEU:HD21	1.91	0.51
1:D:589:LEU:HD13	1:D:589:LEU:H	1.76	0.51
1:B:593:MET:HE1	2:M:2268:ARG:HG2	1.92	0.51
1:B:642:GLN:OE1	3:B:1:486:C32	2.58	0.51
1:D:615:GLN:NE2	1:D:622:CYS:HB3	2.25	0.51
1:B:571:VAL:CG2	3:B:1:486:H283	2.39	0.51
1:B:569:ARG:NH1	1:C:544:LEU:HD22	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:GLY:HA3	1:B:649:VAL:HG22	1.93	0.50
1:C:597:GLN:HG2	1:C:761:ILE:HA	1.94	0.50
1:C:675:VAL:HG13	1:C:772:LEU:HD11	1.94	0.50
1:A:527:MET:O	1:A:528:LEU:CB	2.60	0.50
1:A:579:LYS:HE3	1:B:542:GLU:OE1	2.11	0.49
1:A:725:MET:HA	1:A:728:VAL:HG22	1.93	0.49
1:B:652:GLU:OE2	1:B:655:ARG:NH1	2.46	0.49
1:C:577:TRP:CZ2	1:C:581:ILE:HD11	2.47	0.49
1:D:600:TRP:HA	1:D:603:LEU:HD12	1.94	0.49
1:B:634:MET:CE	1:B:647:LEU:HD11	2.42	0.49
1:B:666:MET:HB3	1:B:722:LEU:HD21	1.95	0.49
1:D:707:ASN:HD22	1:D:710:GLN:NE2	2.11	0.49
1:A:615:GLN:O	1:A:615:GLN:CG	2.58	0.49
1:A:630:ASN:HD21	1:A:632:GLN:HB3	1.78	0.48
1:A:634:MET:CE	1:A:647:LEU:CD1	2.90	0.48
1:C:587:LEU:HD23	1:C:685:LEU:HD23	1.96	0.48
1:C:669:LEU:HD13	1:C:774:PHE:CZ	2.49	0.48
1:D:729:VAL:CG1	1:D:733:LEU:HD22	2.43	0.48
1:A:729:VAL:HG12	1:A:733:LEU:HD22	1.95	0.47
1:B:751:GLU:O	1:B:752:MET:C	2.53	0.47
1:B:530:PRO:CB	1:B:534:SER:HB2	2.43	0.47
1:C:531:THR:HG22	1:C:532:LEU:N	2.29	0.47
1:D:639:MET:HE3	3:D:2:486:C32	2.39	0.47
1:D:570:GLN:HE21	1:D:604:MET:HG2	1.79	0.47
1:A:664:LEU:HD11	1:D:537:GLU:HG3	1.97	0.47
3:A:3:486:HC14	3:A:3:486:HC62	1.75	0.47
1:B:685:LEU:HD22	1:B:685:LEU:O	2.15	0.47
1:A:658:VAL:HG22	1:A:718:LEU:HD21	1.96	0.47
1:C:615:GLN:NE2	1:D:538:VAL:HG13	2.30	0.47
1:A:634:MET:HE3	1:A:647:LEU:HG	1.95	0.47
1:A:629:ILE:HG22	1:A:634:MET:HG3	1.97	0.47
1:A:572:ILE:HG22	1:A:576:LYS:HE2	1.98	0.46
1:A:593:MET:HE1	2:N:2271:LEU:HD12	1.97	0.46
1:A:670:LEU:HD13	1:A:722:LEU:CD2	2.34	0.46
1:C:683:GLN:HE21	1:C:683:GLN:HA	1.81	0.46
1:B:621:LEU:HD11	1:B:646:MET:HB2	1.98	0.46
1:C:563:LEU:HD11	3:C:4:486:H322	1.98	0.46
1:A:751:GLU:HA	1:A:754:ALA:HB3	1.97	0.46
1:A:613:TYR:CE1	1:A:654:HIS:HA	2.51	0.46
1:C:581:ILE:HD13	1:C:668:THR:HG23	1.97	0.46
1:B:572:ILE:HG22	1:B:576:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:MET:HG3	1:C:732:LEU:HD21	1.98	0.46
1:D:587:LEU:HD23	1:D:685:LEU:HD12	1.97	0.46
1:B:761:ILE:N	1:B:762:PRO:HD2	2.32	0.45
1:C:629:ILE:HG23	1:C:633:ARG:CB	2.46	0.45
1:B:571:VAL:HG21	3:B:1:486:C28	2.44	0.45
3:D:2:486:H192	3:D:2:486:C26	2.45	0.45
2:N:2263:LEU:C	2:N:2263:LEU:CD2	2.84	0.45
1:A:691:MET:HB3	1:A:691:MET:HE2	1.73	0.45
1:C:689:ILE:HG23	1:C:693:TYR:HE2	1.81	0.45
1:D:751:GLU:CB	1:D:754:ALA:HB3	2.47	0.45
1:A:527:MET:O	1:A:528:LEU:HB2	2.17	0.45
1:A:554:ASP:OD2	1:D:555:SER:HA	2.16	0.44
1:A:736:CYS:HA	1:A:739:THR:HG22	1.98	0.44
1:C:689:ILE:HG23	1:C:693:TYR:CE2	2.52	0.44
1:C:615:GLN:CD	1:D:538:VAL:HG13	2.38	0.44
1:C:639:MET:CE	3:C:4:486:O3	2.66	0.44
1:B:753:LEU:HB2	3:B:1:486:H293	1.98	0.44
1:C:563:LEU:CD1	3:C:4:486:H322	2.47	0.44
1:D:621:LEU:HD11	1:D:646:MET:HB2	1.99	0.44
1:D:644:LYS:HZ3	1:D:644:LYS:HB2	1.82	0.44
1:D:613:TYR:CE1	1:D:654:HIS:HA	2.53	0.44
3:D:2:486:HC62	3:D:2:486:HC14	1.64	0.44
1:B:760:GLN:O	1:B:763:LYS:HG2	2.18	0.44
1:B:761:ILE:O	1:B:762:PRO:C	2.56	0.44
1:C:615:GLN:CG	1:D:538:VAL:HG13	2.48	0.43
1:C:666:MET:HB3	1:C:722:LEU:HD21	2.00	0.43
1:A:572:ILE:HG21	1:B:538:VAL:HG13	2.01	0.43
2:N:2263:LEU:C	2:N:2263:LEU:HD23	2.39	0.43
1:A:612:SER:O	1:A:616:SER:HB2	2.18	0.43
1:B:610:TRP:HB2	1:B:663:TYR:CE1	2.53	0.43
1:D:608:LEU:HD13	1:D:623:PHE:HA	2.00	0.43
1:C:570:GLN:NE2	3:C:4:486:C2	2.68	0.43
1:C:639:MET:HE3	3:C:4:486:H161	2.00	0.43
1:C:690:ARG:NH1	1:C:694:ILE:HD11	2.33	0.43
1:B:696:GLU:OE2	1:C:533:VAL:HG23	2.19	0.43
1:C:597:GLN:HA	1:C:761:ILE:HG23	2.00	0.42
1:D:671:LEU:HD12	1:D:671:LEU:O	2.19	0.42
1:B:570:GLN:HG2	1:C:544:LEU:HD12	2.02	0.42
1:B:571:VAL:HG22	1:B:604:MET:CE	2.38	0.42
1:D:615:GLN:HG2	5:D:11:HOH:O	2.18	0.42
1:B:571:VAL:HA	1:B:604:MET:HE2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:LEU:N	1:D:544:LEU:HD12	2.34	0.42
1:D:577:TRP:CE2	1:D:581:ILE:HD11	2.54	0.42
1:A:655:ARG:NH2	1:A:656:LEU:HD21	2.34	0.42
1:D:610:TRP:CB	1:D:663:TYR:CE1	3.03	0.42
1:B:638:ASP:O	1:B:642:GLN:NE2	2.52	0.42
1:A:593:MET:HG3	1:A:597:GLN:HE21	1.83	0.42
1:C:672:LEU:HD11	1:C:689:ILE:HG22	2.02	0.42
1:A:609:GLY:HA3	1:A:649:VAL:HG13	2.02	0.42
1:C:617:SER:O	1:C:618:ALA:HB3	2.20	0.42
1:C:652:GLU:O	1:C:656:LEU:HD12	2.19	0.42
1:B:666:MET:SD	1:B:718:LEU:HD22	2.60	0.42
3:C:4:486:HC14	3:C:4:486:HC62	1.65	0.42
1:A:716:TYR:CD2	1:A:716:TYR:C	2.94	0.41
1:B:544:LEU:HD21	1:C:569:ARG:CB	2.49	0.41
1:D:631:GLU:HA	1:D:634:MET:HE2	2.02	0.41
1:A:593:MET:O	1:A:597:GLN:HG3	2.19	0.41
3:A:3:486:HC22	3:A:3:486:H131	1.81	0.41
1:C:634:MET:HE1	1:C:647:LEU:HD11	2.01	0.41
2:N:2263:LEU:HD23	2:N:2263:LEU:O	2.20	0.41
1:C:619:ASN:O	1:C:620:LEU:HD23	2.20	0.41
1:D:621:LEU:HD23	1:D:621:LEU:HA	1.92	0.41
1:A:567:GLY:HA3	3:A:3:486:C25	2.51	0.41
1:B:646:MET:O	1:B:649:VAL:HG13	2.20	0.41
1:A:638:ASP:O	1:A:642:GLN:NE2	2.48	0.41
1:B:646:MET:CE	3:B:1:486:H322	2.51	0.41
1:D:575:VAL:HG22	1:D:596:LEU:HD13	2.03	0.40
1:B:647:LEU:HD23	1:B:647:LEU:HA	1.94	0.40
1:A:749:PHE:CD1	1:A:750:PRO:HD2	2.55	0.40
1:B:724:SER:O	1:B:728:VAL:HG23	2.21	0.40
1:B:555:SER:HB2	1:B:633:ARG:NH2	2.37	0.40
1:B:593:MET:HB2	2:M:2271:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/254 (96%)	222 (91%)	19 (8%)	2 (1%)	19	49
1	B	247/254 (97%)	221 (90%)	22 (9%)	4 (2%)	9	31
1	C	233/254 (92%)	215 (92%)	16 (7%)	2 (1%)	17	46
1	D	228/254 (90%)	214 (94%)	13 (6%)	1 (0%)	34	66
2	M	8/19 (42%)	7 (88%)	1 (12%)	0	100	100
2	N	13/19 (68%)	11 (85%)	2 (15%)	0	100	100
All	All	972/1054 (92%)	890 (92%)	73 (8%)	9 (1%)	17	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	LEU
1	B	769	ILE
1	C	764	TYR
1	D	679	GLY
1	A	530	PRO
1	B	751	GLU
1	C	739	THR
1	B	763	LYS
1	B	706	GLY

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	215/231 (93%)	201 (94%)	14 (6%)	17	44
1	B	219/231 (95%)	202 (92%)	17 (8%)	12	35
1	C	196/231 (85%)	179 (91%)	17 (9%)	10	30
1	D	202/231 (87%)	187 (93%)	15 (7%)	13	37
2	M	7/15 (47%)	5 (71%)	2 (29%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	10/15 (67%)	8 (80%)	2 (20%)	1 4
All	All	849/954 (89%)	782 (92%)	67 (8%)	12 34

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	VAL
1	A	535	LEU
1	A	551	SER
1	A	595	LEU
1	A	633	ARG
1	A	642	GLN
1	A	652	GLU
1	A	663	TYR
1	A	667	LYS
1	A	670	LEU
1	A	716	TYR
1	A	733	LEU
1	A	734	ASN
1	A	760	GLN
1	B	534	SER
1	B	537	GLU
1	B	555	SER
1	B	585	ARG
1	B	595	LEU
1	B	621	LEU
1	B	627	LEU
1	B	633	ARG
1	B	649	VAL
1	B	674	SER
1	B	683	GLN
1	B	685	LEU
1	B	691	MET
1	B	704	ARG
1	B	763	LYS
1	B	766	ASN
1	B	776	GLN
1	C	535	LEU
1	C	558	ARG
1	C	595	LEU
1	C	613	TYR
1	C	615	GLN

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Mol	Chain	Res	Type
1	C	639	MET
1	C	640	TYR
1	C	670	LEU
1	C	674	SER
1	C	683	GLN
1	C	711	ASN
1	C	733	LEU
1	C	734	ASN
1	C	755	GLU
1	C	756	ILE
1	C	763	LYS
1	C	776	GLN
1	D	535	LEU
1	D	576	LYS
1	D	585	ARG
1	D	589	LEU
1	D	595	LEU
1	D	627	LEU
1	D	636	LEU
1	D	677	LYS
1	D	683	GLN
1	D	685	LEU
1	D	728	VAL
1	D	733	LEU
1	D	752	MET
1	D	758	THR
1	D	776	GLN
2	N	2263	LEU
2	N	2272	MET
2	M	2269	LYS
2	M	2272	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	570	GLN
1	A	586	ASN
1	A	597	GLN
1	A	619	ASN
1	A	760	GLN
1	B	570	GLN
1	B	586	ASN

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Mol	Chain	Res	Type
1	B	615	GLN
1	B	683	GLN
1	B	711	ASN
1	B	731	ASN
1	B	776	GLN
1	C	570	GLN
1	C	683	GLN
1	C	710	GLN
1	C	711	ASN
1	C	734	ASN
1	D	570	GLN
1	D	615	GLN
1	D	707	ASN
1	D	711	ASN
1	D	768	ASN
1	D	775	HIS
1	D	776	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	486	B	1	-	36,36,36	0.84	2 (5%)	52,56,56	2.10	11 (21%)
3	486	C	4	-	36,36,36	0.72	1 (2%)	52,56,56	1.89	10 (19%)
4	GOL	B	778	-	5,5,5	0.36	0	5,5,5	0.56	0
3	486	D	2	-	36,36,36	0.81	1 (2%)	52,56,56	1.90	11 (21%)
3	486	A	3	-	36,36,36	0.61	0	52,56,56	1.57	9 (17%)

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	486	B	1	-	-	0/8/72/72	0/5/5/5
3	486	C	4	-	-	0/8/72/72	0/5/5/5
4	GOL	B	778	-	-	2/4/4/4	-
3	486	D	2	-	-	2/8/72/72	0/5/5/5
3	486	A	3	-	-	2/8/72/72	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1	486	C12-C17	-2.73	1.51	1.56
3	D	2	486	C12-C17	-2.41	1.52	1.56
3	B	1	486	C3-C2	-2.30	1.40	1.45
3	C	4	486	C12-C17	-2.14	1.52	1.56

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1	486	C12-C11-C9	-8.23	106.35	113.50
3	C	4	486	C12-C11-C9	-6.75	107.63	113.50
3	D	2	486	C12-C11-C9	-6.57	107.79	113.50
3	B	1	486	C16-C17-C12	-5.58	98.45	102.85
3	A	3	486	C12-C11-C9	-5.58	108.65	113.50
3	D	2	486	C19-C12-C17	4.99	112.57	108.00
3	C	4	486	C6-C5-C10	-4.62	119.21	123.82
3	C	4	486	C13-C12-C11	4.25	111.80	108.03
3	B	1	486	C13-C12-C11	4.24	111.79	108.03
3	B	1	486	C1-C2-C3	3.99	122.89	116.74
3	D	2	486	C1-C2-C3	3.90	122.75	116.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	4	486	C18-C14-C10	-3.79	106.09	112.88
3	B	1	486	C6-C5-C10	-3.79	120.04	123.82
3	D	2	486	C6-C5-C10	-3.55	120.28	123.82
3	C	4	486	C1-C2-C3	3.42	122.00	116.74
3	D	2	486	C19-C12-C13	-3.41	106.40	111.11
3	C	4	486	C16-C17-C12	3.25	105.41	102.85
3	D	2	486	C12-C17-C31	-3.23	107.42	111.14
3	A	3	486	C1-C2-C3	3.23	121.72	116.74
3	B	1	486	C15-C11-C9	-3.02	113.36	118.15
3	A	3	486	C15-C11-C9	-2.95	113.47	118.15
3	B	1	486	C17-C12-C11	-2.90	98.03	100.03
3	A	3	486	C18-C14-C10	-2.88	107.73	112.88
3	A	3	486	C6-C5-C10	-2.77	121.05	123.82
3	B	1	486	C15-C16-C17	-2.71	104.15	106.65
3	A	3	486	C19-C12-C17	2.70	110.47	108.00
3	B	1	486	C2-C3-C4	-2.64	120.53	122.87
3	C	4	486	C19-C12-C17	2.59	110.37	108.00
3	D	2	486	C15-C16-C17	-2.54	104.31	106.65
3	D	2	486	C15-C11-C9	-2.51	114.16	118.15
3	C	4	486	C13-C12-C17	-2.50	112.81	115.83
3	A	3	486	C15-C16-C17	-2.48	104.37	106.65
3	A	3	486	C8-C7-C4	-2.45	105.65	111.07
3	B	1	486	C8-C7-C4	-2.39	105.79	111.07
3	B	1	486	C18-C14-C10	-2.27	108.82	112.88
3	A	3	486	C17-C12-C11	-2.14	98.55	100.03
3	D	2	486	C25-C24-N27	-2.07	118.83	121.63
3	C	4	486	C11-C9-C10	-2.07	104.24	108.85
3	C	4	486	C15-C11-C12	-2.04	101.00	103.73
3	D	2	486	O3-C17-C31	2.03	111.60	108.09
3	D	2	486	C23-C22-C18	-2.00	119.18	121.20

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	778	GOL	O1-C1-C2-C3
4	B	778	GOL	O1-C1-C2-O2
3	A	3	486	C13-C14-C18-C22
3	A	3	486	C13-C14-C18-C26
3	D	2	486	C13-C14-C18-C22
3	D	2	486	C13-C14-C18-C26

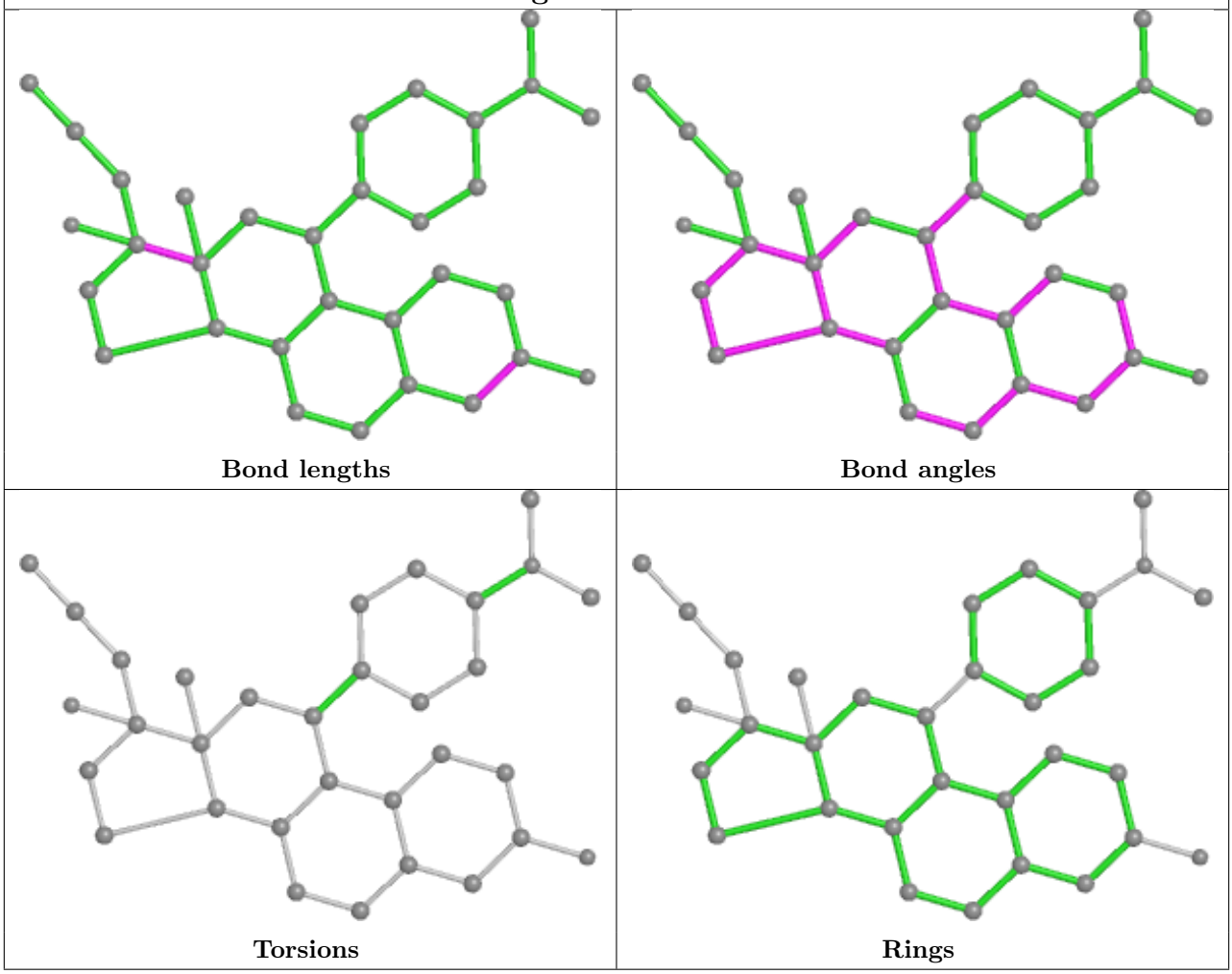
There are no ring outliers.

4 monomers are involved in 35 short contacts:

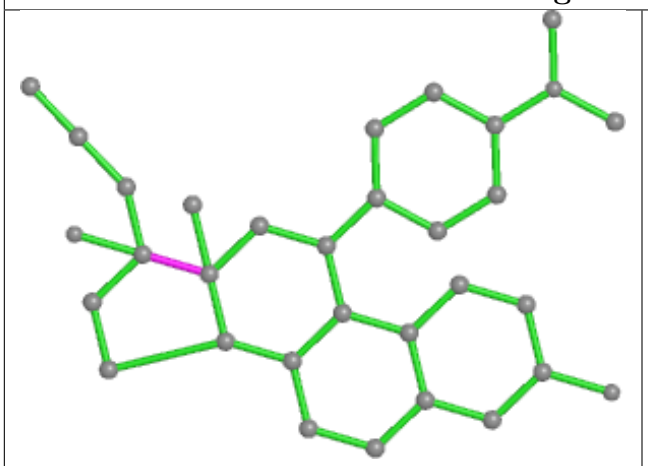
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1	486	9	0
3	C	4	486	7	0
3	D	2	486	14	0
3	A	3	486	5	0

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.

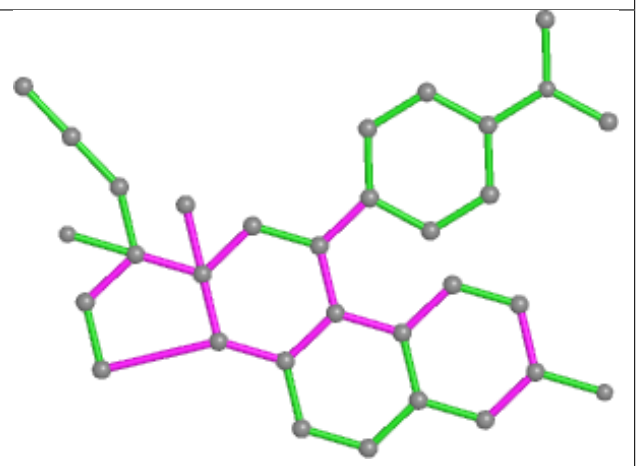
Ligand 486 B 1



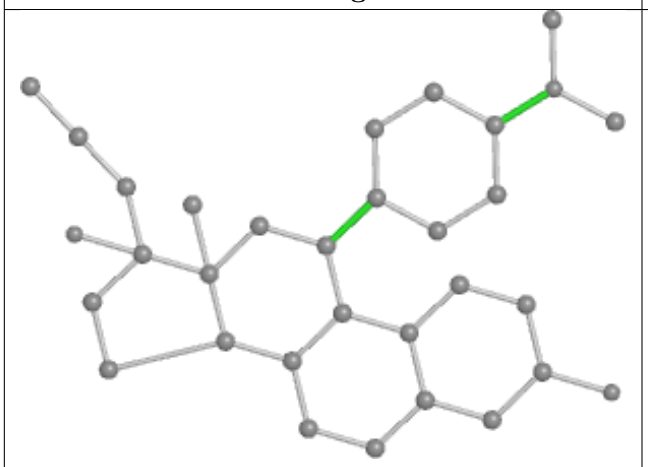
Ligand 486 C 4



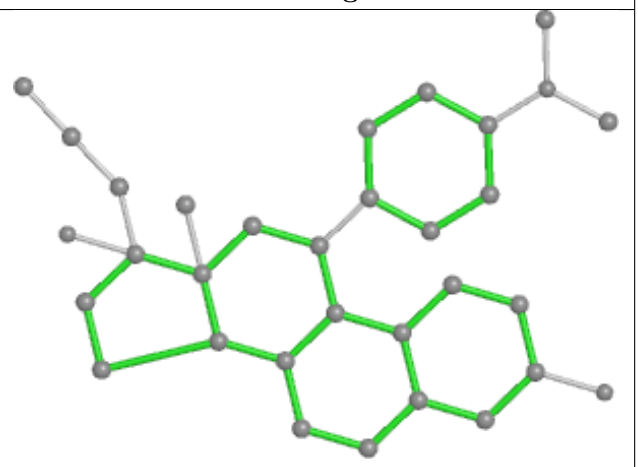
Bond lengths



Bond angles

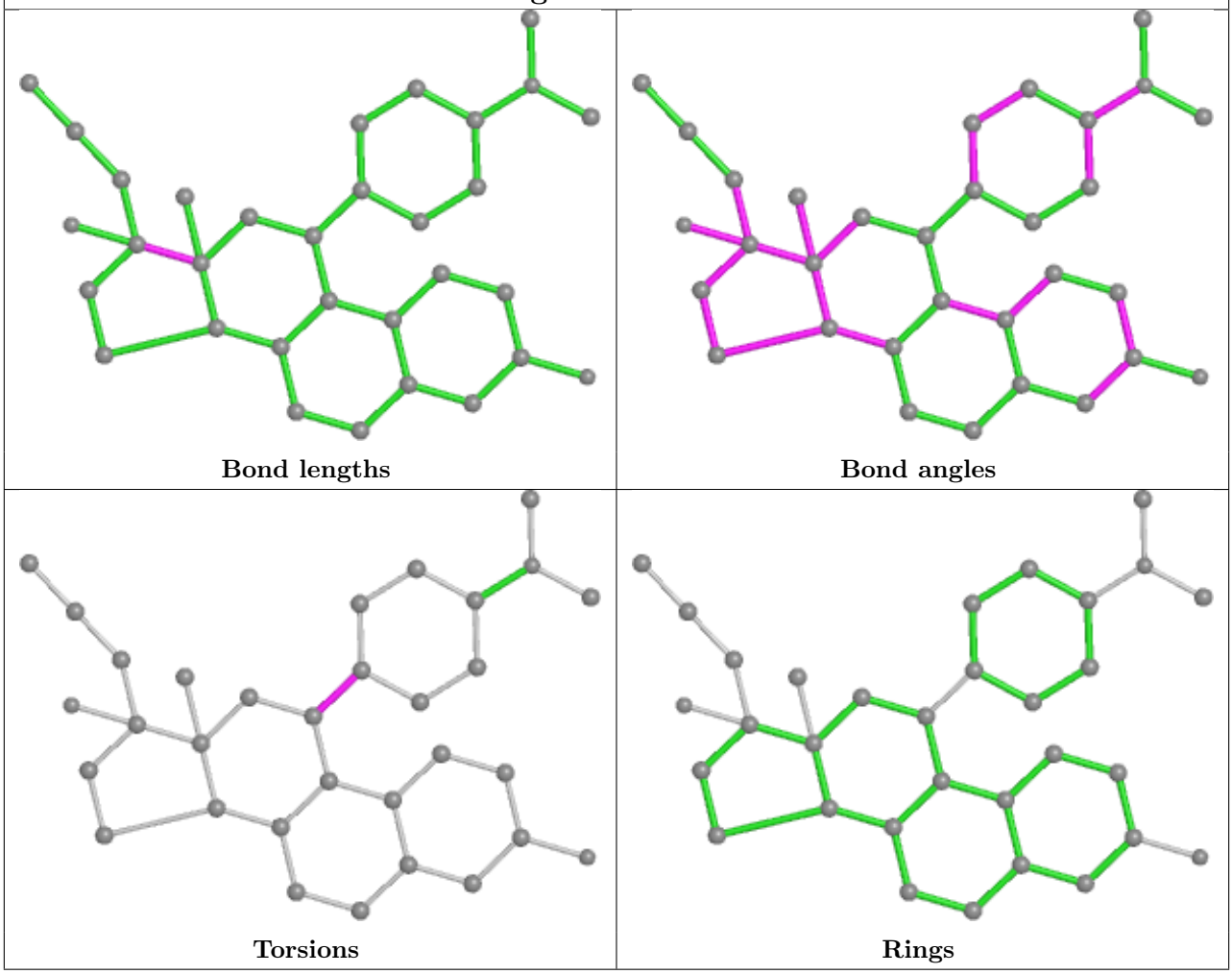


Torsions

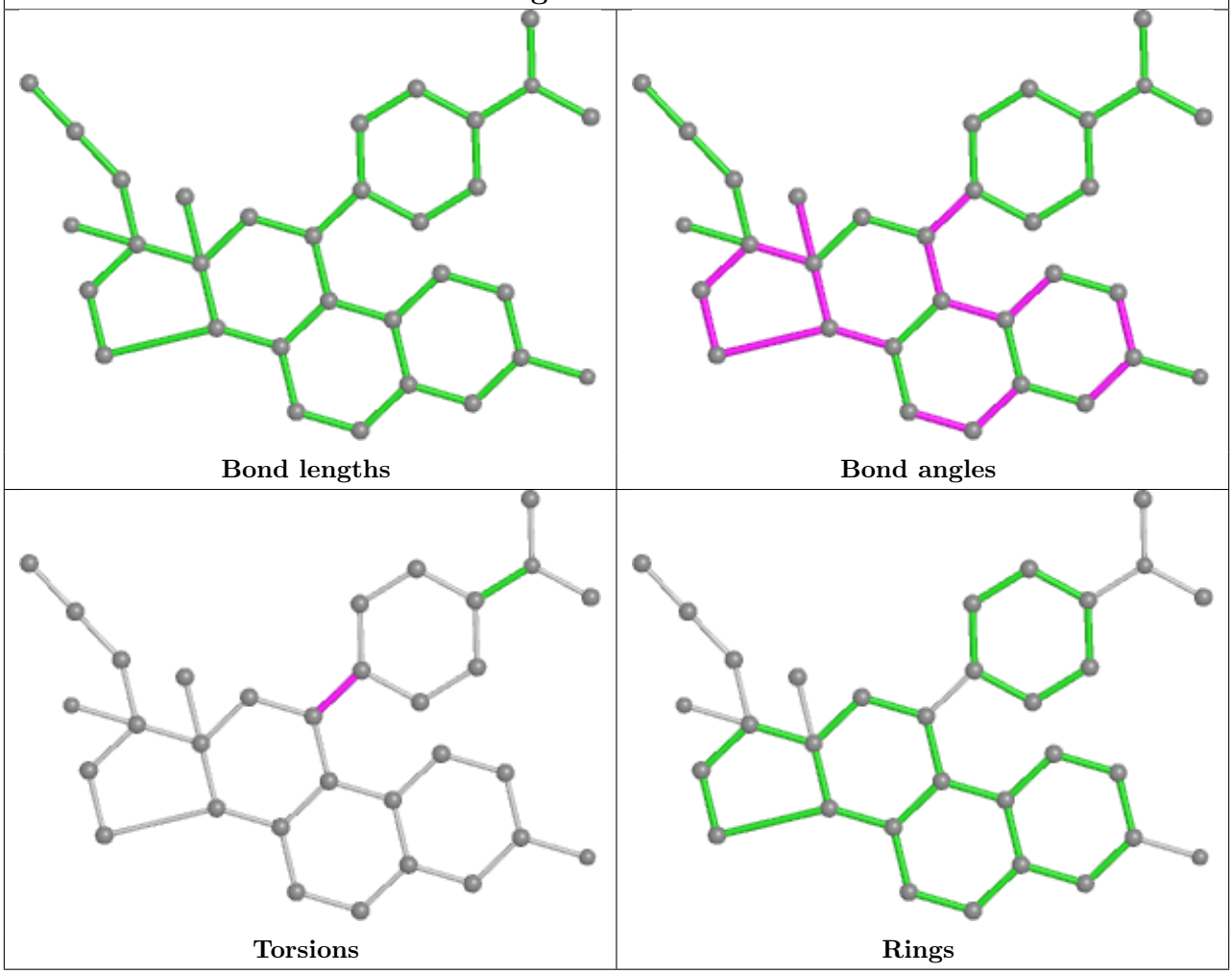


Rings

Ligand 486 D 2



Ligand 486 A 3



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	247/254 (97%)	-0.26	2 (0%)	86	81	33, 43, 69, 76	0
1	B	249/254 (98%)	-0.35	5 (2%)	65	56	37, 47, 69, 75	0
1	C	237/254 (93%)	-0.04	6 (2%)	57	47	34, 50, 69, 80	0
1	D	234/254 (92%)	-0.25	4 (1%)	70	63	25, 43, 55, 74	0
2	M	10/19 (52%)	-0.18	0	100	100	32, 34, 37, 38	0
2	N	15/19 (78%)	-0.28	1 (6%)	17	10	45, 50, 58, 58	0
All	All	992/1054 (94%)	-0.23	18 (1%)	68	61	25, 46, 68, 80	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	635	THR	7.2
1	D	739	THR	3.8
1	C	637	PRO	3.2
1	C	764	TYR	2.9
1	B	711	ASN	2.8
1	C	636	LEU	2.7
1	C	754	ALA	2.6
1	B	528	LEU	2.5
1	B	776	GLN	2.5
1	B	764	TYR	2.5
1	A	741	LEU	2.3
1	A	760	GLN	2.3
1	D	707	ASN	2.2
1	D	766	ASN	2.2
2	N	2260	ASN	2.2
1	D	741	LEU	2.2
1	B	765	SER	2.1
1	C	634	MET	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

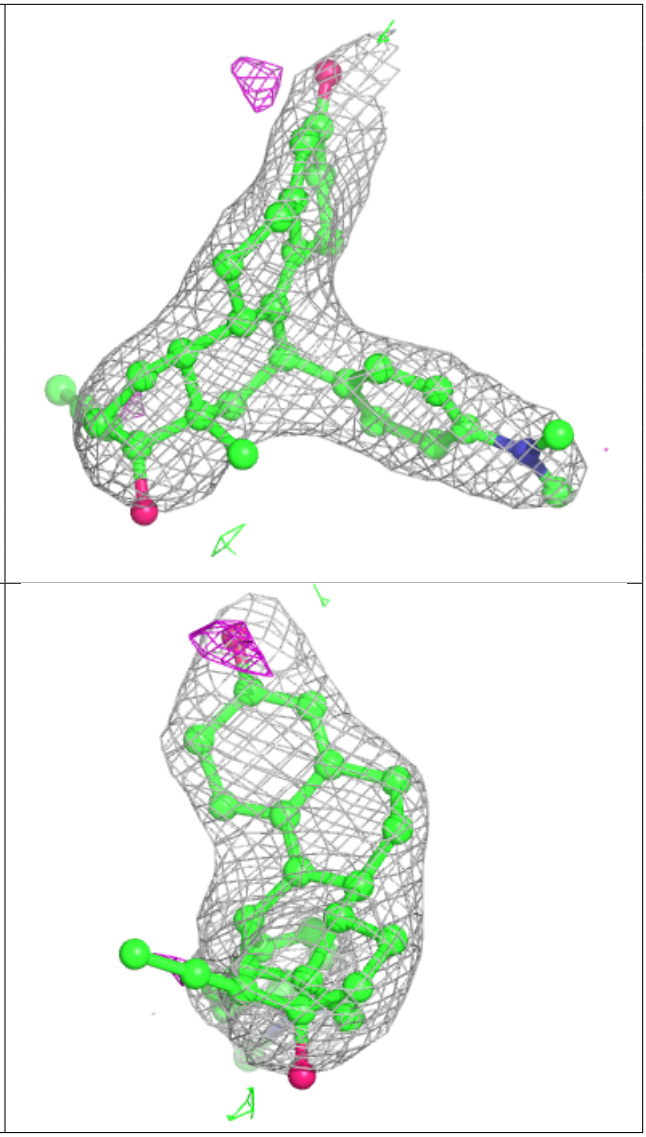
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	B	778	6/6	0.91	0.11	80,80,81,81	0
3	486	C	4	32/32	0.95	0.26	43,48,54,54	0
3	486	D	2	32/32	0.96	0.15	31,34,35,36	0
3	486	B	1	32/32	0.96	0.18	29,40,43,45	0
3	486	A	3	32/32	0.97	0.22	32,39,41,41	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.

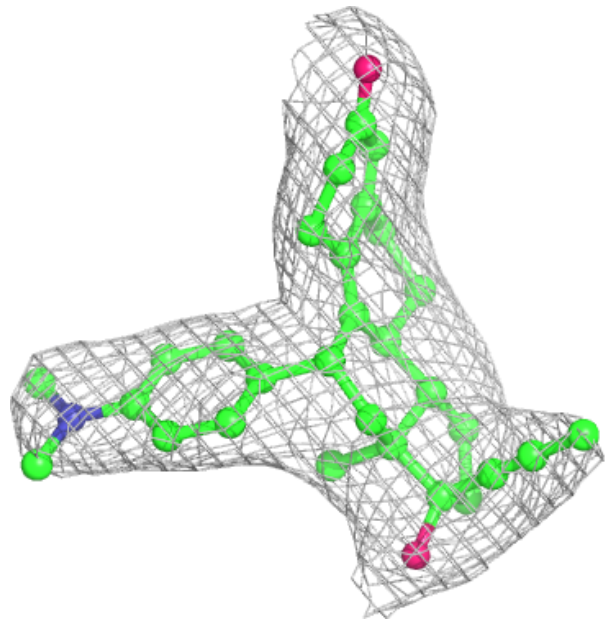
Electron density around 486 C 4:

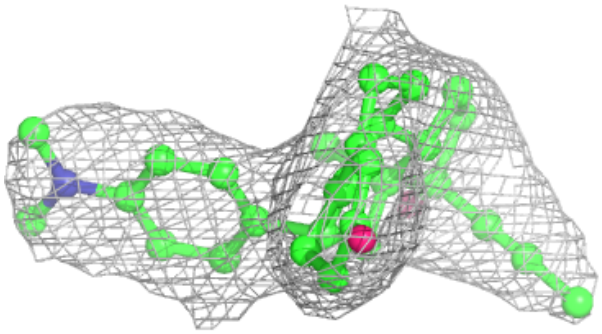
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

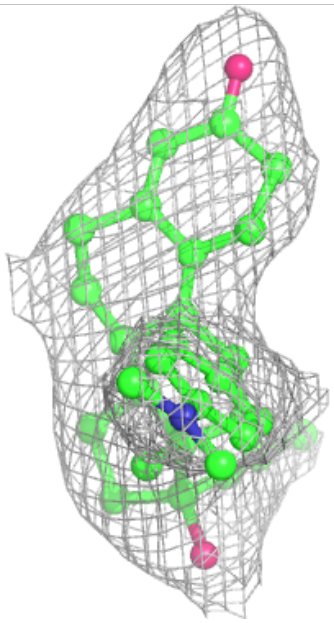


Electron density around 486 D 2:

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

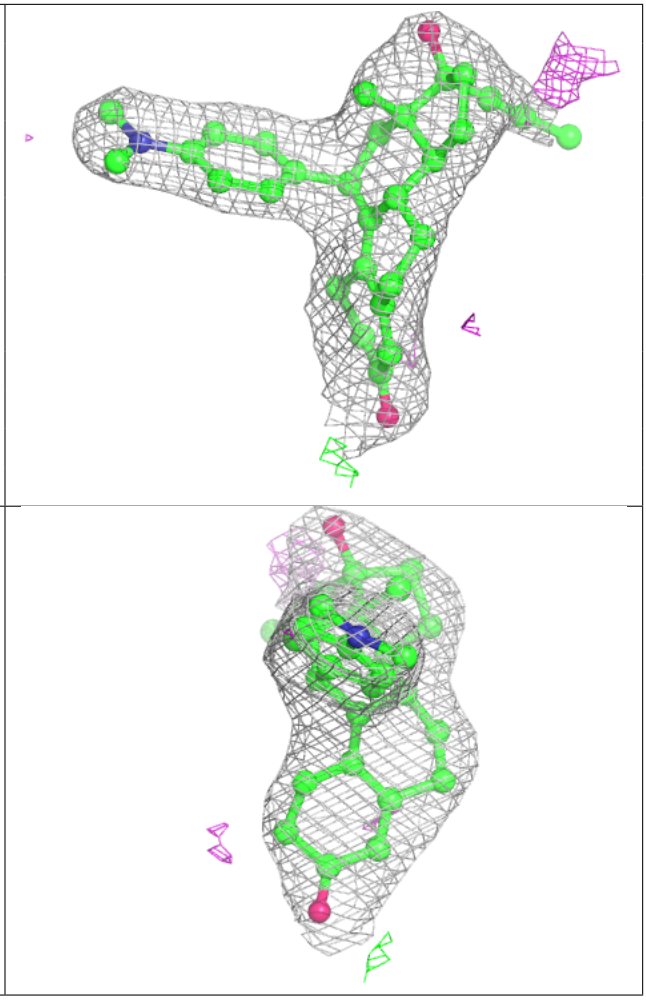






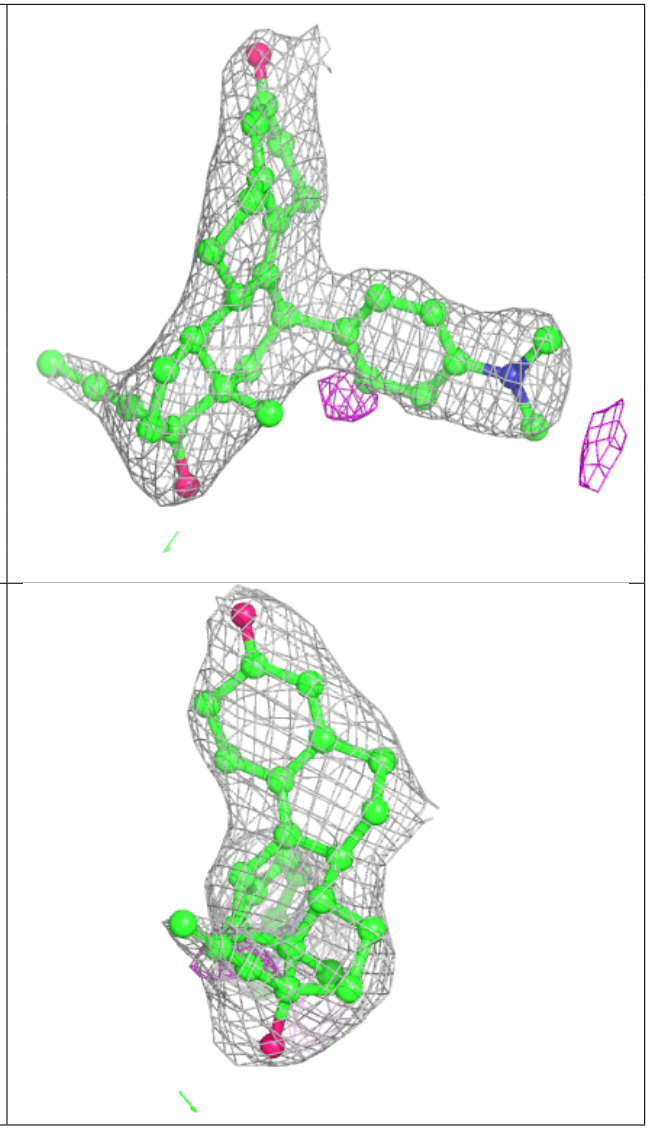
Electron density around 486 B 1:

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



Electron density around 486 A 3:

$2mF_o$-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.