Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 04:35 AM EDT

PDB ID	:	1YA3
Title	:	Crystal structure of the human mineralocorticoid receptor ligand-binding domain bound to progesterone and harboring the S810L mutation responsible for a severe form of hypertension
Authors	:	Fagart, J.; Huyet, J.; Pinon, G.M.; Rochel, M.; Mayer, C.; Rafestin-Oblin, M.E.
Deposited on	:	2004-12-17
Resolution	:	2.34 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 (1)) were used in the production of this report:

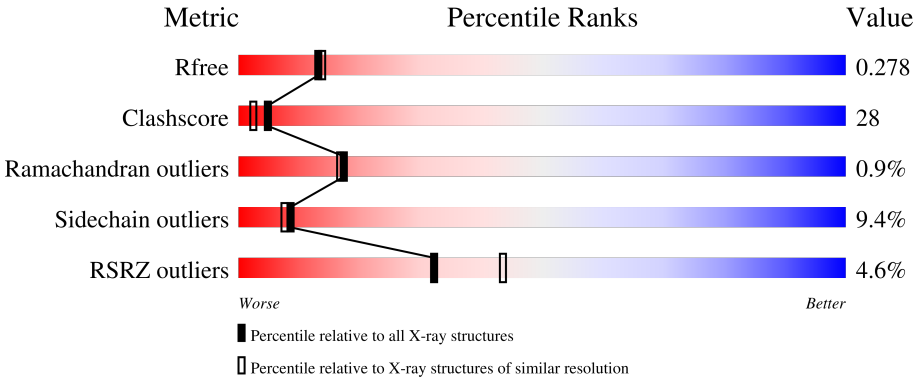
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	255	5% 52% 33% 6% 9%
1	B	255	4% 49% 37% • 10%
1	C	255	4% 45% 38% 7% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	STR	C	3001	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5764 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.

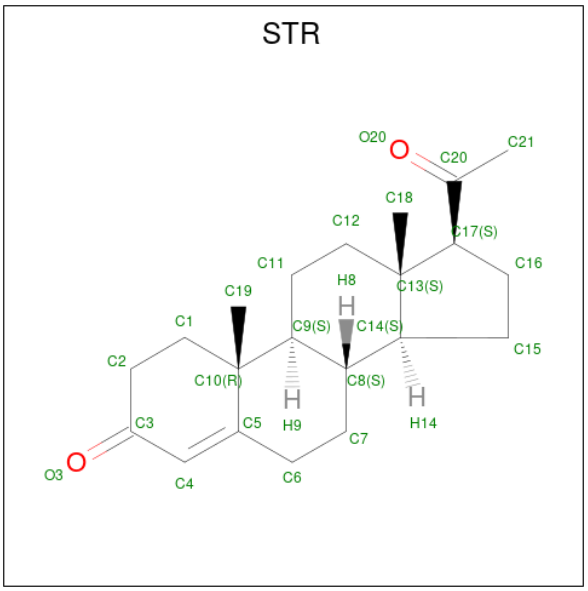
- Molecule 1 is a protein called Mineralocorticoid receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1890	1235	301	340	14			
1	B	230	Total	C	N	O	S	0	0	0
			1860	1215	296	335	14			
1	C	232	Total	C	N	O	S	0	0	0
			1888	1231	301	342	14			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	730	SER	-	cloning artifact	UNP P08235
A	810	LEU	SER	engineered mutation	UNP P08235
A	910	ALA	CYS	engineered mutation	UNP P08235
B	730	SER	-	cloning artifact	UNP P08235
B	810	LEU	SER	engineered mutation	UNP P08235
B	910	ALA	CYS	engineered mutation	UNP P08235
C	730	SER	-	cloning artifact	UNP P08235
C	810	LEU	SER	engineered mutation	UNP P08235
C	910	ALA	CYS	engineered mutation	UNP P08235

- Molecule 2 is PROGESTERONE (three-letter code: STR) (formula: $C_{21}H_{30}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 23 21 2	0	0
2	B	1	Total C O 23 21 2	0	0
2	C	1	Total C O 23 21 2	0	0

- Molecule 3 is water.

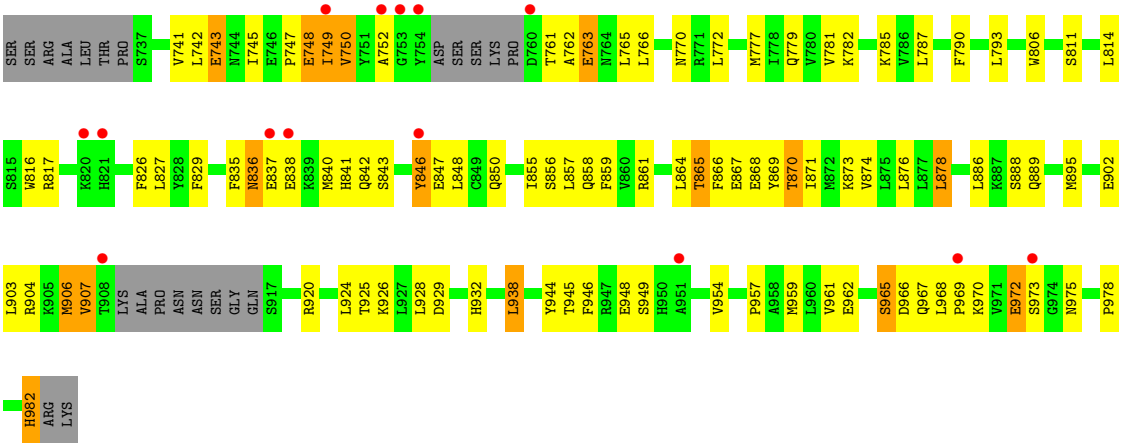
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	0	0
3	B	10	Total O 10 10	0	0
3	C	25	Total O 25 25	0	0

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.

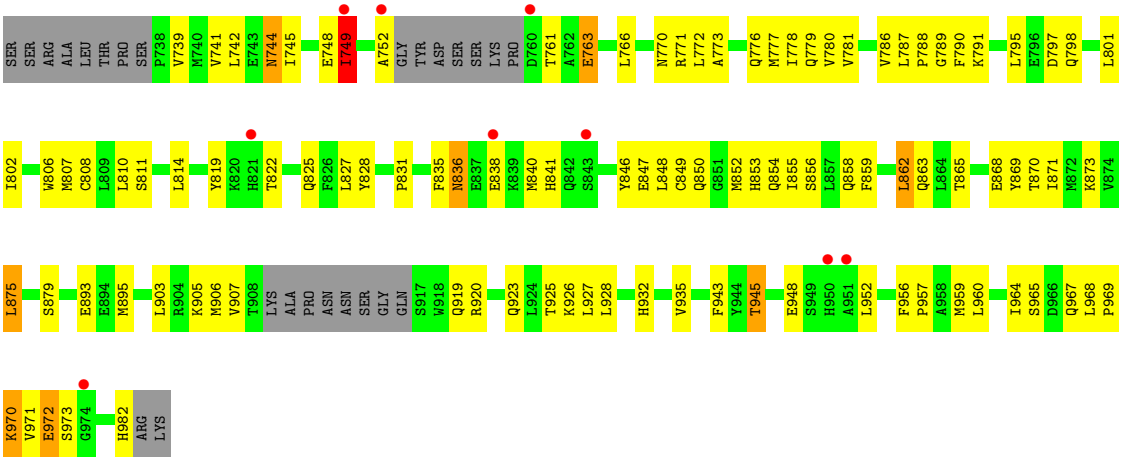
• Molecule 1: Mineralocorticoid receptor

Chain A:



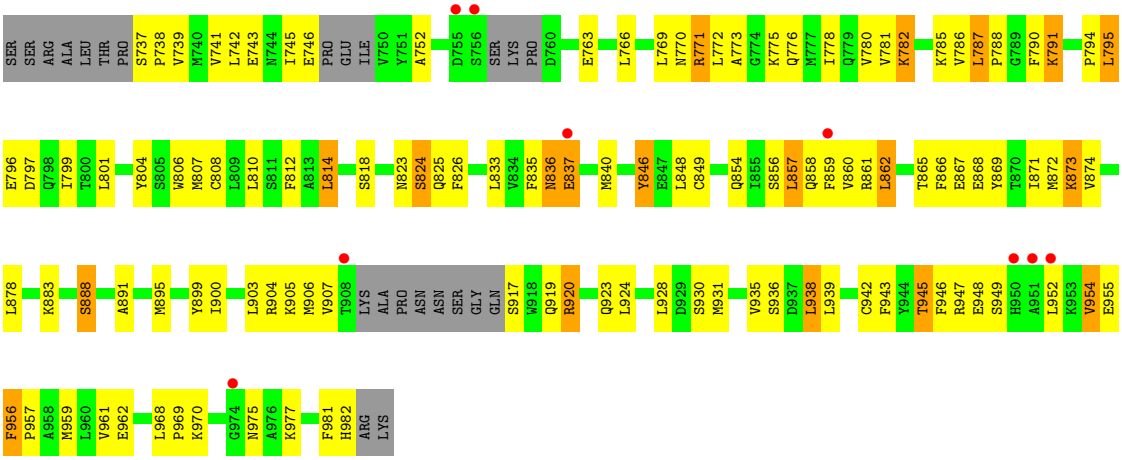
• Molecule 1: Mineralocorticoid receptor

Chain B:



• Molecule 1: Mineralocorticoid receptor

Chain C:


SER SER ARG ALA LEU THR PRO S737 P738 V739 M740 V741 L742 E743 N744 I745 E746 PRO GLU ILE V750 Y751 A752 D755 S756 SER LYS PRO D760 E763 L766 L769 N770 R771 L772 A773 G774 K775 Q776 M777 I778 Q779 V780 V781 K782 K785 V786 L787 P788 G789 F790 K791 P794 L795
E796 D797 Q798 I799 T800 L801 Y804 S805 W806 M807 C808 L809 L810 S811 F812 A813 L814 S818 N823 S824 Q825 F826 L833 V834 F835 N836 E837 M840 Y846 E847 L848 C849 Q854 I855 S856 L857 Q858 F859 V860 R861 L862 T865 F866 E867 E868 Y869 T870 I871 M872 K873 V874
L878 K883 S888 A891 M895 Y899 I900 L903 R904 K905 M906 V907 T908 LYS ALA PRO ASN ASN SER GLY GLN S917 W918 Q919 R920 Q923 L924 L928 D929 S930 M931 V935 S936 D937 L938 L939 C942 F943 Y944 T945 F946 R947 E948 S949 H950 A951 L952 K953 V954 E955
F956 P957 A958 M959 L960 V961 E962 L968 P969 K970 G974 N975 A976 K977 F981 H982 ARG LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	120.72Å 120.72Å 42.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.72 – 2.34 18.72 – 2.34	Depositor EDS
% Data completeness (in resolution range)	81.7 (18.72-2.34) 76.1 (18.72-2.34)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.35Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.237 , 0.284 0.223 , 0.278	Depositor DCC
R_{free} test set	2186 reflections (9.15%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.774	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l 0.047 for h,-h-k,-l 0.024 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5764	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9363e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: STR

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	0.61	2/1934 (0.1%)	0.71	2/2619 (0.1%)
1	B	0.42	1/1904 (0.1%)	0.63	2/2581 (0.1%)
1	C	0.49	2/1931 (0.1%)	0.66	2/2611 (0.1%)
All	All	0.51	5/5769 (0.1%)	0.66	6/7811 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	973	SER	C-N	-15.79	1.04	1.33
1	A	982	HIS	C-O	-7.57	1.08	1.23
1	B	982	HIS	C-O	-7.05	1.09	1.23
1	C	982	HIS	C-O	7.02	1.36	1.23
1	C	956	PHE	C-N	-6.42	1.22	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	982	HIS	CA-C-O	8.22	137.37	120.10
1	C	846	TYR	N-CA-C	7.20	130.45	111.00
1	A	846	TYR	N-CA-C	5.63	126.22	111.00
1	B	846	TYR	N-CA-C	5.20	125.03	111.00
1	B	982	HIS	CA-C-O	5.16	130.94	120.10
1	C	956	PHE	O-C-N	-5.05	111.50	121.10

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	1890	0	1872	103	1
1	B	1860	0	1834	84	0
1	C	1888	0	1867	128	2
2	A	23	0	30	1	0
2	B	23	0	30	2	0
2	C	23	0	30	12	0
3	A	22	0	0	0	0
3	B	10	0	0	1	0
3	C	25	0	0	1	0
All	All	5764	0	5663	315	3

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 28.

All (315) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:LYS:O	1:C:791:LYS:HD3	1.19	1.32
1:A:836:ASN:ND2	1:A:837:GLU:H	1.55	1.02
1:C:771:ARG:HD2	1:C:957:PRO:HG3	1.04	1.02
1:C:771:ARG:CD	1:C:957:PRO:HG3	1.90	1.01
1:A:836:ASN:HD22	1:A:837:GLU:H	1.09	0.96
1:C:907:VAL:HG13	1:C:920:ARG:HD2	1.44	0.96
1:A:781:VAL:O	1:A:785:LYS:HG2	1.64	0.96
1:B:806:TRP:HE1	1:B:967:GLN:HE22	1.17	0.92
1:C:771:ARG:HH12	1:C:955:GLU:HB3	1.34	0.91
1:C:785:LYS:O	1:C:791:LYS:CD	2.15	0.90
1:C:771:ARG:HD2	1:C:957:PRO:CG	2.00	0.86
1:B:943:PHE:CG	1:B:968:LEU:HD13	2.11	0.85
1:B:948:GLU:HB3	1:B:952:LEU:HD13	1.60	0.83
1:C:807:MET:HE1	2:C:3001:STR:H72	1.59	0.83
1:C:846:TYR:O	1:C:846:TYR:CD1	2.32	0.82
1:A:836:ASN:HD22	1:A:837:GLU:N	1.78	0.82
1:A:836:ASN:ND2	1:A:837:GLU:N	2.28	0.81
1:C:904:ARG:HG2	1:C:904:ARG:HH21	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:846:TYR:O	1:C:846:TYR:CG	2.35	0.79
1:B:798:GLN:O	1:B:802:ILE:HG13	1.83	0.79
1:A:846:TYR:CD1	1:A:846:TYR:O	2.36	0.79
1:B:865:THR:N	1:B:868:GLU:OE1	2.13	0.79
1:A:827:LEU:HB2	1:A:835:PHE:HB2	1.63	0.78
1:A:817:ARG:NH1	1:A:829:PHE:O	2.19	0.76
1:A:742:LEU:HD13	1:A:870:THR:HG23	1.67	0.76
1:A:782:LYS:HA	1:A:785:LYS:HD3	1.68	0.76
1:C:771:ARG:NH1	1:C:955:GLU:HB3	2.00	0.75
1:C:883:LYS:HZ2	1:C:975:ASN:HA	1.50	0.75
1:B:787:LEU:HD12	1:B:788:PRO:HD2	1.68	0.74
1:B:766:LEU:HD22	2:B:2001:STR:H213	1.70	0.74
1:A:752:ALA:HB2	1:A:772:LEU:HD13	1.69	0.73
1:C:745:ILE:HD12	1:C:786:VAL:HG23	1.70	0.73
1:B:970:LYS:HE3	1:B:970:LYS:HA	1.72	0.72
1:A:846:TYR:O	1:A:846:TYR:CG	2.43	0.72
1:A:972:GLU:O	1:A:975:ASN:ND2	2.23	0.72
1:B:773:ALA:HB3	1:B:960:LEU:HD21	1.70	0.71
1:B:822:THR:O	1:B:825:GLN:HG3	1.91	0.71
1:C:752:ALA:HB2	1:C:772:LEU:HD22	1.73	0.70
1:C:883:LYS:NZ	1:C:975:ASN:HA	2.06	0.70
1:A:749:ILE:O	1:A:750:VAL:HG23	1.92	0.70
1:C:766:LEU:HD22	2:C:3001:STR:H213	1.73	0.70
1:A:777:MET:O	1:A:781:VAL:HG23	1.92	0.69
1:A:920:ARG:NH1	1:A:924:LEU:HD21	2.07	0.69
1:C:907:VAL:CG1	1:C:920:ARG:HD2	2.21	0.69
1:C:737:SER:HB3	1:C:738:PRO:HD3	1.75	0.69
1:C:787:LEU:O	1:C:791:LYS:HB2	1.92	0.69
1:B:739:VAL:HG21	1:B:906:MET:HE1	1.75	0.69
1:B:865:THR:OG1	1:B:868:GLU:HG3	1.93	0.69
1:B:945:THR:HG22	1:B:956:PHE:HZ	1.57	0.69
1:B:967:GLN:O	1:B:971:VAL:HG23	1.94	0.68
1:C:904:ARG:HG2	1:C:904:ARG:NH2	2.07	0.68
1:C:771:ARG:HA	1:C:957:PRO:HG3	1.75	0.67
1:B:836:ASN:O	1:B:840:MET:HG3	1.95	0.66
1:C:807:MET:HE1	2:C:3001:STR:C7	2.26	0.66
1:C:771:ARG:HA	1:C:957:PRO:CG	2.26	0.65
1:C:865:THR:OG1	1:C:867:GLU:HG2	1.96	0.65
1:A:742:LEU:CD1	1:A:870:THR:CG2	2.74	0.65
1:B:849:CYS:HA	1:B:852:MET:HE3	1.77	0.65
1:A:920:ARG:HH12	1:A:924:LEU:HD21	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:LEU:HB2	1:A:969:PRO:HD3	1.78	0.65
1:B:919:GLN:O	1:B:923:GLN:HG3	1.97	0.65
1:B:761:THR:OG1	1:B:763:GLU:HG2	1.97	0.64
1:C:878:LEU:HD21	1:C:895:MET:CE	2.28	0.64
1:A:747:PRO:HB3	1:A:779:GLN:HB3	1.79	0.64
1:B:806:TRP:HE1	1:B:967:GLN:NE2	1.95	0.63
1:C:812:PHE:HD2	1:C:873:LYS:HG2	1.62	0.63
1:C:867:GLU:OE1	1:C:906:MET:HB3	1.99	0.63
1:B:859:PHE:HE1	1:B:927:LEU:HD21	1.63	0.63
1:A:865:THR:HG22	1:A:868:GLU:H	1.64	0.63
1:C:770:ASN:HB3	1:C:957:PRO:HD3	1.80	0.63
1:C:920:ARG:HA	1:C:923:GLN:HE21	1.63	0.62
1:C:867:GLU:HG3	1:C:868:GLU:N	2.15	0.62
1:A:926:LYS:HD2	1:A:982:HIS:CD2	2.35	0.62
1:A:846:TYR:CD1	1:A:846:TYR:C	2.73	0.62
1:A:749:ILE:O	1:A:750:VAL:CG2	2.48	0.62
1:A:946:PHE:HE1	1:A:961:VAL:HG22	1.65	0.62
1:A:945:THR:CG2	1:A:954:VAL:HG11	2.30	0.61
1:B:925:THR:HA	1:B:928:LEU:HD12	1.82	0.61
1:C:804:TYR:OH	1:C:970:LYS:CE	2.49	0.61
1:C:928:LEU:O	1:C:931:MET:HB2	2.01	0.61
1:A:787:LEU:HD23	1:A:790:PHE:CB	2.30	0.61
1:C:807:MET:CE	2:C:3001:STR:H72	2.30	0.61
1:A:761:THR:OG1	1:A:763:GLU:HG2	2.01	0.60
1:A:945:THR:HG22	1:A:954:VAL:HG11	1.82	0.60
1:A:926:LYS:HD2	1:A:982:HIS:HD2	1.66	0.60
1:A:857:LEU:O	1:A:861:ARG:HG3	2.01	0.60
1:A:907:VAL:CG1	1:A:920:ARG:HB3	2.32	0.60
1:B:749:ILE:O	1:B:749:ILE:CD1	2.49	0.60
1:A:742:LEU:HD13	1:A:870:THR:CG2	2.32	0.59
1:B:945:THR:HG22	1:B:956:PHE:CZ	2.36	0.59
1:A:742:LEU:CD1	1:A:870:THR:HG23	2.32	0.59
1:C:737:SER:CB	1:C:738:PRO:HD3	2.31	0.59
1:A:855:ILE:O	1:A:858:GLN:HB2	2.03	0.59
1:B:970:LYS:HA	1:B:970:LYS:CE	2.31	0.59
1:B:741:VAL:HG13	1:B:742:LEU:N	2.18	0.59
1:C:807:MET:CE	2:C:3001:STR:C7	2.80	0.59
1:C:947:ARG:C	1:C:948:GLU:HG2	2.23	0.59
1:C:848:LEU:HD22	1:C:938:LEU:HD12	1.85	0.58
1:A:876:LEU:HD21	1:A:928:LEU:HD23	1.86	0.58
1:B:749:ILE:CD1	1:B:749:ILE:C	2.71	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:LEU:HD12	1:B:814:LEU:O	2.02	0.58
1:B:741:VAL:O	1:B:745:ILE:HG13	2.04	0.57
1:C:900:ILE:HG12	1:C:981:PHE:HE1	1.67	0.57
1:C:739:VAL:O	1:C:743:GLU:HG3	2.03	0.57
1:C:840:MET:SD	1:C:849:CYS:HB3	2.44	0.57
1:C:812:PHE:CD2	1:C:873:LYS:HG2	2.39	0.57
1:C:770:ASN:O	1:C:957:PRO:HG2	2.04	0.57
1:C:858:GLN:O	1:C:862:LEU:HB2	2.04	0.57
1:A:765:LEU:HD11	1:A:835:PHE:HZ	1.70	0.57
1:A:961:VAL:O	1:A:965:SER:HB2	2.05	0.56
1:C:846:TYR:CD1	1:C:846:TYR:C	2.77	0.56
1:C:952:LEU:N	1:C:952:LEU:HD22	2.21	0.56
1:A:743:GLU:HB3	1:A:866:PHE:HE2	1.70	0.56
1:C:814:LEU:O	1:C:814:LEU:CD2	2.54	0.56
1:A:766:LEU:HD22	2:A:1001:STR:H213	1.87	0.56
1:C:857:LEU:O	1:C:861:ARG:HG3	2.06	0.56
1:B:847:GLU:HA	1:B:850:GLN:HB2	1.87	0.56
1:C:857:LEU:O	1:C:860:VAL:HG12	2.06	0.56
1:B:827:LEU:HG	1:B:840:MET:HE1	1.89	0.55
1:A:962:GLU:O	1:A:966:ASP:OD2	2.24	0.55
1:B:776:GLN:O	1:B:779:GLN:HG2	2.06	0.55
1:C:878:LEU:HD21	1:C:895:MET:HE3	1.89	0.55
1:A:954:VAL:O	1:A:954:VAL:HG13	2.05	0.55
1:C:883:LYS:NZ	1:C:883:LYS:HB3	2.22	0.55
1:A:864:LEU:HD12	1:A:868:GLU:OE2	2.06	0.55
1:B:749:ILE:O	1:B:749:ILE:HD12	2.07	0.55
1:A:742:LEU:HB3	1:A:870:THR:HG23	1.87	0.55
1:C:818:SER:HB3	1:C:826:PHE:O	2.07	0.55
1:C:907:VAL:CG1	1:C:920:ARG:HB3	2.37	0.54
1:A:907:VAL:HG13	1:A:920:ARG:HB3	1.89	0.54
1:C:945:THR:HG21	2:C:3001:STR:H211	1.89	0.54
1:A:932:HIS:CE1	1:A:978:PRO:HB3	2.42	0.54
1:C:770:ASN:ND2	2:C:3001:STR:H121	2.23	0.54
1:B:770:ASN:HB3	1:B:957:PRO:HD3	1.89	0.54
1:A:748:GLU:O	1:A:750:VAL:HG23	2.08	0.54
1:C:795:LEU:CD1	1:C:799:ILE:HD13	2.38	0.54
1:C:888:SER:HB2	1:C:891:ALA:HB3	1.89	0.54
1:C:814:LEU:CD2	1:C:814:LEU:C	2.76	0.54
1:B:790:PHE:N	1:B:895:MET:SD	2.81	0.53
1:C:787:LEU:HD12	1:C:788:PRO:HD2	1.89	0.53
1:A:907:VAL:O	1:A:907:VAL:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:LEU:HD13	1:A:861:ARG:HH21	1.72	0.53
1:B:773:ALA:CB	1:B:960:LEU:HD21	2.37	0.53
1:B:742:LEU:HD22	1:B:870:THR:HB	1.89	0.53
1:B:776:GLN:O	1:B:780:VAL:HG23	2.08	0.52
1:A:878:LEU:CD1	1:A:878:LEU:N	2.73	0.52
1:A:765:LEU:HD11	1:A:835:PHE:CZ	2.44	0.52
1:B:787:LEU:HD12	1:B:788:PRO:CD	2.39	0.52
1:A:742:LEU:HB3	1:A:870:THR:CG2	2.39	0.52
1:B:968:LEU:O	1:B:972:GLU:HB2	2.10	0.52
1:A:749:ILE:C	1:A:750:VAL:HG23	2.30	0.52
1:C:769:LEU:HB3	2:C:3001:STR:H112	1.90	0.52
1:A:743:GLU:HB3	1:A:866:PHE:CE2	2.46	0.51
1:B:739:VAL:HG21	1:B:906:MET:CE	2.39	0.51
1:C:790:PHE:HE1	1:C:801:LEU:HD12	1.75	0.51
1:A:816:TRP:HB2	1:A:869:TYR:CE1	2.45	0.51
1:B:945:THR:HG21	2:B:2001:STR:H211	1.92	0.51
1:B:777:MET:O	1:B:781:VAL:HG23	2.10	0.51
1:A:836:ASN:O	1:A:840:MET:HG3	2.10	0.51
1:C:807:MET:CE	2:C:3001:STR:H8	2.40	0.51
1:B:752:ALA:HA	1:B:772:LEU:HD13	1.92	0.51
1:B:772:LEU:O	1:B:776:GLN:HG3	2.10	0.51
1:C:807:MET:HE3	2:C:3001:STR:H8	1.92	0.51
1:C:797:ASP:OD2	1:C:888:SER:OG	2.28	0.50
1:C:823:ASN:O	1:C:824:SER:HB2	2.11	0.50
1:A:742:LEU:HD12	1:A:870:THR:CG2	2.41	0.50
1:A:752:ALA:CB	1:A:772:LEU:HD13	2.40	0.50
1:A:763:GLU:CD	1:A:763:GLU:H	2.14	0.50
1:A:765:LEU:HD23	1:A:843:SER:HB3	1.94	0.50
1:B:770:ASN:O	1:B:957:PRO:HG2	2.12	0.50
1:A:806:TRP:HE1	1:A:967:GLN:NE2	2.10	0.50
1:A:944:TYR:CE1	1:A:948:GLU:HG3	2.47	0.50
1:B:797:ASP:O	1:B:801:LEU:HD23	2.12	0.50
1:C:814:LEU:O	1:C:814:LEU:HD23	2.12	0.49
1:C:919:GLN:O	1:C:923:GLN:HG3	2.12	0.49
1:B:808:CYS:HA	1:B:935:VAL:HG21	1.94	0.49
1:C:946:PHE:HE1	1:C:961:VAL:HG22	1.77	0.49
1:C:949:SER:HB2	1:C:954:VAL:O	2.13	0.49
1:A:870:THR:HG22	1:A:871:ILE:N	2.28	0.49
1:A:925:THR:HA	1:A:928:LEU:HD12	1.94	0.49
1:A:765:LEU:HD21	1:A:835:PHE:CZ	2.48	0.49
1:A:865:THR:HG22	1:A:867:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:ILE:O	1:B:749:ILE:HD13	2.13	0.48
1:B:776:GLN:HE21	1:B:810:LEU:HD22	1.78	0.48
1:B:806:TRP:CG	1:B:807:MET:N	2.81	0.48
1:B:969:PRO:O	1:B:973:SER:HB3	2.14	0.48
1:C:782:LYS:NZ	3:C:4029:HOH:O	2.45	0.48
1:C:808:CYS:SG	1:C:935:VAL:HG21	2.53	0.48
1:C:952:LEU:H	1:C:952:LEU:CD2	2.25	0.48
1:C:848:LEU:HD22	1:C:938:LEU:CD1	2.44	0.48
1:A:761:THR:HB	1:A:763:GLU:OE1	2.13	0.48
1:A:929:ASP:O	1:A:932:HIS:HB2	2.14	0.48
1:A:787:LEU:HD11	1:A:874:VAL:HG22	1.96	0.47
1:B:903:LEU:O	1:B:907:VAL:HG23	2.14	0.47
1:C:737:SER:O	1:C:741:VAL:HG13	2.14	0.47
1:C:807:MET:CE	2:C:3001:STR:H62	2.44	0.47
1:A:869:TYR:OH	1:A:873:LYS:HE2	2.14	0.47
1:B:741:VAL:HG11	1:B:788:PRO:HG2	1.96	0.47
1:A:907:VAL:HG11	1:A:920:ARG:HB3	1.96	0.47
1:C:801:LEU:HD13	1:C:878:LEU:HD23	1.96	0.47
1:B:827:LEU:HB2	1:B:835:PHE:HB2	1.97	0.47
1:C:878:LEU:CD2	1:C:895:MET:CE	2.93	0.47
1:A:793:LEU:HG	1:A:895:MET:HE1	1.96	0.47
1:C:771:ARG:HA	1:C:957:PRO:HG2	1.97	0.47
1:C:804:TYR:CZ	1:C:970:LYS:HE2	2.49	0.47
1:B:749:ILE:C	1:B:749:ILE:HD13	2.34	0.47
1:C:867:GLU:HG3	1:C:868:GLU:HG3	1.97	0.47
1:B:848:LEU:O	1:B:852:MET:HG3	2.15	0.46
1:A:765:LEU:CD2	1:A:843:SER:HB3	2.45	0.46
1:A:770:ASN:HB3	1:A:957:PRO:HD3	1.98	0.46
1:A:871:ILE:HD12	1:A:906:MET:HG3	1.97	0.46
1:A:949:SER:HA	1:A:954:VAL:HG12	1.97	0.46
1:C:770:ASN:HB3	1:C:957:PRO:CD	2.45	0.46
1:C:814:LEU:C	1:C:814:LEU:HD22	2.36	0.46
1:A:811:SER:O	1:A:814:LEU:HB3	2.16	0.46
1:C:806:TRP:O	1:C:810:LEU:HG	2.16	0.46
1:C:737:SER:CB	1:C:738:PRO:CD	2.94	0.46
1:C:770:ASN:O	1:C:773:ALA:HB3	2.16	0.46
1:A:874:VAL:O	1:A:878:LEU:HD13	2.15	0.45
1:C:741:VAL:HG21	1:C:788:PRO:CG	2.47	0.45
1:C:952:LEU:N	1:C:952:LEU:CD2	2.79	0.45
1:B:787:LEU:O	1:B:791:LYS:HG2	2.16	0.45
1:B:858:GLN:O	1:B:862:LEU:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:TYR:OH	1:B:873:LYS:HD3	2.17	0.45
1:C:741:VAL:HG22	1:C:742:LEU:N	2.31	0.45
1:A:886:LEU:H	1:A:889:GLN:HE21	1.63	0.45
1:C:872:MET:HG2	1:C:928:LEU:HD11	1.97	0.45
1:C:883:LYS:NZ	1:C:883:LYS:CB	2.78	0.45
1:C:814:LEU:O	1:C:814:LEU:HD22	2.15	0.45
1:A:782:LYS:HA	1:A:785:LYS:CD	2.43	0.45
1:B:879:SER:HB2	1:B:932:HIS:HE1	1.82	0.45
1:B:875:LEU:HD12	1:B:875:LEU:HA	1.78	0.45
1:C:948:GLU:O	1:C:952:LEU:HD23	2.16	0.45
1:B:871:ILE:HD11	1:B:906:MET:HE3	1.98	0.45
1:A:742:LEU:CB	1:A:870:THR:HG21	2.47	0.44
1:B:859:PHE:CE1	1:B:927:LEU:HD21	2.49	0.44
1:B:907:VAL:HG13	1:B:920:ARG:HG2	1.99	0.44
1:C:871:ILE:CD1	1:C:906:MET:HG3	2.47	0.44
1:C:946:PHE:HA	1:C:956:PHE:CE1	2.52	0.44
1:A:782:LYS:O	1:A:785:LYS:HG3	2.17	0.44
1:B:850:GLN:O	1:B:854:GLN:HG2	2.17	0.44
1:A:848:LEU:HD22	1:A:938:LEU:HD13	2.00	0.44
1:C:878:LEU:HD11	1:C:895:MET:HE3	1.98	0.44
1:C:794:PRO:HD2	1:C:888:SER:OG	2.17	0.44
1:C:796:GLU:CD	1:C:796:GLU:H	2.21	0.44
1:C:874:VAL:HG11	1:C:899:TYR:CE1	2.53	0.44
1:C:900:ILE:HG12	1:C:981:PHE:CE1	2.51	0.44
1:C:969:PRO:HG2	1:C:970:LYS:H	1.83	0.44
1:B:862:LEU:O	1:B:863:GLN:HB2	2.18	0.44
1:B:776:GLN:NE2	3:B:4034:HOH:O	2.50	0.44
1:B:905:LYS:HA	1:B:905:LYS:HD2	1.84	0.44
1:C:836:ASN:ND2	1:C:837:GLU:H	2.16	0.44
1:A:742:LEU:CB	1:A:870:THR:CG2	2.96	0.43
1:A:878:LEU:N	1:A:878:LEU:HD13	2.33	0.43
1:B:744:ASN:C	1:B:744:ASN:HD22	2.21	0.43
1:C:804:TYR:OH	1:C:970:LYS:NZ	2.51	0.43
1:C:782:LYS:O	1:C:785:LYS:CG	2.66	0.43
1:C:943:PHE:CD1	1:C:968:LEU:HD12	2.53	0.43
1:A:865:THR:CG2	1:A:867:GLU:H	2.31	0.43
1:B:943:PHE:CB	1:B:968:LEU:HD13	2.48	0.43
1:A:856:SER:O	1:A:859:PHE:HB2	2.18	0.43
1:C:907:VAL:HG11	1:C:920:ARG:HB3	1.99	0.43
1:A:762:ALA:HA	1:A:842:GLN:O	2.18	0.43
1:B:827:LEU:HG	1:B:840:MET:CE	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:ILE:HB	1:C:786:VAL:HG21	2.01	0.43
1:C:787:LEU:HB3	1:C:790:PHE:HB3	1.99	0.43
1:B:771:ARG:HA	1:B:957:PRO:HG3	2.01	0.43
1:C:943:PHE:HB3	1:C:968:LEU:HD12	2.01	0.43
1:A:749:ILE:H	1:A:749:ILE:HG13	1.55	0.43
1:C:952:LEU:HD22	1:C:952:LEU:H	1.83	0.42
1:A:848:LEU:HD23	1:A:848:LEU:HA	1.92	0.42
1:B:778:ILE:HG22	1:B:779:GLN:N	2.34	0.42
1:A:787:LEU:HD23	1:A:790:PHE:CG	2.54	0.42
1:A:816:TRP:CH2	1:A:866:PHE:HA	2.54	0.42
1:A:826:PHE:HB3	1:A:835:PHE:O	2.19	0.42
1:A:903:LEU:O	1:A:906:MET:HB2	2.19	0.42
1:B:838:GLU:O	1:B:841:HIS:HB2	2.19	0.42
1:A:787:LEU:HD23	1:A:790:PHE:HB3	2.00	0.42
1:A:838:GLU:O	1:A:841:HIS:HB2	2.18	0.42
1:B:741:VAL:CG1	1:B:742:LEU:N	2.83	0.42
1:B:855:ILE:HD12	1:B:927:LEU:HD11	2.02	0.42
1:C:942:CYS:HA	2:C:3001:STR:O20	2.19	0.42
1:C:869:TYR:OH	1:C:873:LYS:HE3	2.19	0.42
1:C:935:VAL:O	1:C:939:LEU:HG	2.19	0.42
1:C:746:GLU:HG2	1:C:866:PHE:HZ	1.84	0.42
1:B:960:LEU:O	1:B:964:ILE:HG13	2.20	0.41
1:C:883:LYS:HB3	1:C:883:LYS:HZ3	1.85	0.41
1:A:966:ASP:O	1:A:970:LYS:HD3	2.20	0.41
1:C:947:ARG:O	1:C:948:GLU:HG2	2.21	0.41
1:C:968:LEU:N	1:C:969:PRO:HD2	2.35	0.41
1:A:742:LEU:HB2	1:A:870:THR:HG21	2.03	0.41
1:C:778:ILE:O	1:C:781:VAL:HG12	2.20	0.41
1:C:848:LEU:HD23	1:C:848:LEU:HA	1.90	0.41
1:C:903:LEU:O	1:C:907:VAL:HG23	2.20	0.41
1:A:886:LEU:H	1:A:889:GLN:NE2	2.18	0.41
1:B:741:VAL:HG22	1:B:745:ILE:HD11	2.03	0.41
1:C:905:LYS:HB3	1:C:905:LYS:HE3	1.79	0.41
1:C:867:GLU:CG	1:C:868:GLU:N	2.82	0.41
1:A:741:VAL:O	1:A:745:ILE:HG12	2.20	0.41
1:A:949:SER:HA	1:A:954:VAL:CG1	2.50	0.41
1:B:828:TYR:OH	1:B:831:PRO:HA	2.20	0.41
1:B:853:HIS:O	1:B:856:SER:HB3	2.20	0.41
1:C:752:ALA:HA	1:C:772:LEU:HD13	2.02	0.41
1:C:836:ASN:O	1:C:840:MET:HG3	2.20	0.41
1:A:748:GLU:O	1:A:749:ILE:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:771:ARG:HD2	1:C:771:ARG:HA	1.61	0.41
1:C:833:LEU:HD11	1:C:835:PHE:HE1	1.85	0.41
1:C:878:LEU:HD21	1:C:895:MET:HE1	2.03	0.41
1:B:741:VAL:HG13	1:B:742:LEU:H	1.86	0.40
1:B:819:TYR:CD1	1:B:859:PHE:HB3	2.57	0.40
1:A:816:TRP:CZ2	1:A:866:PHE:HD1	2.39	0.40
1:B:787:LEU:HA	1:B:788:PRO:HD3	1.85	0.40
1:B:789:GLY:C	1:B:895:MET:SD	3.00	0.40
1:C:776:GLN:O	1:C:780:VAL:HG23	2.21	0.40
1:C:856:SER:O	1:C:859:PHE:HB2	2.20	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:825:GLN:NE2	1:C:970:LYS:NZ[1_554]	2.00	0.20
1:C:804:TYR:OH	1:C:825:GLN:OE1[1_556]	2.11	0.09
1:A:902:GLU:OE2	1:A:962:GLU:OE2[3_764]	2.13	0.07

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	227/255 (89%)	206 (91%)	16 (7%)	5 (2%)	6 4
1	B	224/255 (88%)	218 (97%)	5 (2%)	1 (0%)	34 38
1	C	224/255 (88%)	209 (93%)	15 (7%)	0	100 100
All	All	675/765 (88%)	633 (94%)	36 (5%)	6 (1%)	17 17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	749	ILE
1	A	749	ILE
1	A	907	VAL
1	A	906	MET
1	A	972	GLU
1	A	750	VAL

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	207/234 (88%)	193 (93%)	14 (7%)	16 17
1	B	204/234 (87%)	187 (92%)	17 (8%)	11 11
1	C	208/234 (89%)	181 (87%)	27 (13%)	4 3
All	All	619/702 (88%)	561 (91%)	58 (9%)	8 7

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	743	GLU
1	A	748	GLU
1	A	763	GLU
1	A	836	ASN
1	A	847	GLU
1	A	850	GLN
1	A	865	THR
1	A	870	THR
1	A	878	LEU
1	A	888	SER
1	A	904	ARG
1	A	938	LEU
1	A	959	MET
1	A	965	SER
1	B	744	ASN
1	B	748	GLU
1	B	749	ILE

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Mol	Chain	Res	Type
1	B	763	GLU
1	B	786	VAL
1	B	795	LEU
1	B	811	SER
1	B	836	ASN
1	B	862	LEU
1	B	875	LEU
1	B	893	GLU
1	B	926	LYS
1	B	945	THR
1	B	959	MET
1	B	965	SER
1	B	970	LYS
1	B	972	GLU
1	C	763	GLU
1	C	771	ARG
1	C	775	LYS
1	C	782	LYS
1	C	787	LEU
1	C	791	LYS
1	C	795	LEU
1	C	814	LEU
1	C	824	SER
1	C	836	ASN
1	C	837	GLU
1	C	854	GLN
1	C	857	LEU
1	C	862	LEU
1	C	873	LYS
1	C	888	SER
1	C	917	SER
1	C	920	ARG
1	C	924	LEU
1	C	930	SER
1	C	936	SER
1	C	938	LEU
1	C	945	THR
1	C	954	VAL
1	C	959	MET
1	C	962	GLU
1	C	977	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	764	ASN
1	A	836	ASN
1	A	850	GLN
1	A	853	HIS
1	A	889	GLN
1	A	898	ASN
1	A	932	HIS
1	A	967	GLN
1	A	975	ASN
1	B	744	ASN
1	B	764	ASN
1	B	776	GLN
1	B	854	GLN
1	B	932	HIS
1	B	967	GLN
1	C	770	ASN
1	C	776	GLN
1	C	825	GLN
1	C	836	ASN
1	C	898	ASN
1	C	923	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)

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	$\#\|Z\| > 2$
2	STR	B	2001	-	26,26,26	5.05	15 (57%)	42,42,42	1.80	9 (21%)
2	STR	A	1001	-	26,26,26	4.19	14 (53%)	42,42,42	1.64	11 (26%)
2	STR	C	3001	-	26,26,26	4.73	20 (76%)	42,42,42	1.62	9 (21%)

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
2	STR	B	2001	-	-	0/4/62/62	0/4/4/4
2	STR	A	1001	-	-	0/4/62/62	0/4/4/4
2	STR	C	3001	-	-	0/4/62/62	0/4/4/4

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	STR	C4-C5	12.03	1.52	1.34
2	C	3001	STR	C4-C5	10.88	1.50	1.34
2	A	1001	STR	C4-C5	9.34	1.48	1.34
2	B	2001	STR	C12-C13	9.16	1.70	1.54
2	B	2001	STR	C10-C5	8.74	1.70	1.52
2	C	3001	STR	C8-C9	8.67	1.70	1.53
2	B	2001	STR	C19-C10	8.65	1.69	1.54
2	B	2001	STR	C18-C13	8.40	1.69	1.54
2	B	2001	STR	C8-C9	8.01	1.68	1.53
2	C	3001	STR	C10-C5	7.23	1.67	1.52
2	A	1001	STR	C8-C9	7.18	1.67	1.53
2	C	3001	STR	C12-C13	7.12	1.66	1.54
2	C	3001	STR	C11-C9	7.12	1.65	1.53
2	A	1001	STR	C1-C10	6.74	1.67	1.54
2	A	1001	STR	C18-C13	6.69	1.66	1.54
2	C	3001	STR	C6-C5	6.67	1.62	1.50
2	A	1001	STR	C6-C5	6.57	1.61	1.50
2	A	1001	STR	C12-C13	6.14	1.65	1.54
2	B	2001	STR	C11-C9	6.01	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	STR	C8-C14	5.97	1.65	1.53
2	C	3001	STR	C18-C13	5.39	1.63	1.54
2	A	1001	STR	C10-C5	5.10	1.63	1.52
2	A	1001	STR	C11-C9	5.08	1.62	1.53
2	A	1001	STR	C13-C14	4.93	1.64	1.55
2	C	3001	STR	C17-C20	4.40	1.58	1.51
2	C	3001	STR	C1-C2	4.30	1.62	1.53
2	A	1001	STR	C19-C10	4.18	1.61	1.54
2	C	3001	STR	O20-C20	4.13	1.32	1.21
2	C	3001	STR	C13-C14	3.83	1.62	1.55
2	C	3001	STR	C7-C6	3.82	1.61	1.52
2	C	3001	STR	C13-C17	3.74	1.62	1.56
2	B	2001	STR	C1-C10	3.72	1.61	1.54
2	A	1001	STR	C7-C8	3.68	1.60	1.53
2	C	3001	STR	C1-C10	3.49	1.60	1.54
2	C	3001	STR	C7-C8	3.27	1.59	1.53
2	B	2001	STR	C6-C5	3.26	1.56	1.50
2	C	3001	STR	C10-C9	3.24	1.61	1.56
2	A	1001	STR	C13-C17	-3.23	1.50	1.56
2	B	2001	STR	C15-C14	3.21	1.61	1.54
2	B	2001	STR	C17-C20	3.16	1.56	1.51
2	B	2001	STR	C13-C14	3.05	1.60	1.55
2	C	3001	STR	C21-C20	2.85	1.57	1.49
2	C	3001	STR	C4-C3	2.55	1.51	1.45
2	A	1001	STR	C10-C9	2.54	1.60	1.56
2	B	2001	STR	C21-C20	2.48	1.56	1.49
2	B	2001	STR	C2-C3	2.22	1.54	1.49
2	A	1001	STR	O20-C20	2.19	1.27	1.21
2	C	3001	STR	C2-C3	2.16	1.54	1.49
2	C	3001	STR	C16-C15	2.12	1.59	1.54

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	STR	C17-C13-C14	-4.91	94.49	99.72
2	B	2001	STR	C2-C3-C4	4.18	123.18	116.74
2	B	2001	STR	C5-C4-C3	-4.04	117.16	123.67
2	A	1001	STR	C2-C3-C4	3.96	122.84	116.74
2	C	3001	STR	C2-C3-C4	3.92	122.78	116.74
2	C	3001	STR	C19-C10-C5	-3.60	102.52	108.34
2	A	1001	STR	C15-C14-C13	3.59	108.17	103.84
2	B	2001	STR	C6-C7-C8	3.58	118.18	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3001	STR	C13-C17-C20	3.47	119.87	114.98
2	A	1001	STR	C17-C13-C14	-3.20	96.31	99.72
2	B	2001	STR	C21-C20-C17	3.05	121.99	117.56
2	B	2001	STR	O3-C3-C2	-2.91	115.55	121.57
2	B	2001	STR	C13-C17-C20	2.81	118.93	114.98
2	C	3001	STR	O3-C3-C2	-2.75	115.88	121.57
2	A	1001	STR	C11-C9-C8	2.57	115.46	111.75
2	A	1001	STR	O20-C20-C17	-2.51	117.80	121.69
2	C	3001	STR	C2-C1-C10	2.49	118.13	113.45
2	A	1001	STR	C16-C15-C14	-2.46	100.26	105.13
2	B	2001	STR	C13-C14-C8	-2.44	110.77	114.38
2	A	1001	STR	C13-C17-C20	2.41	118.38	114.98
2	A	1001	STR	C21-C20-C17	2.37	121.01	117.56
2	C	3001	STR	C7-C8-C14	2.28	115.98	112.08
2	A	1001	STR	C18-C13-C17	2.20	113.81	110.24
2	C	3001	STR	C15-C14-C13	2.16	106.45	103.84
2	B	2001	STR	C1-C10-C9	2.16	111.74	108.73
2	A	1001	STR	C15-C16-C17	2.13	108.80	105.30
2	A	1001	STR	C18-C13-C14	2.09	115.61	111.71
2	C	3001	STR	C6-C7-C8	2.09	115.47	111.69
2	C	3001	STR	C18-C13-C12	2.00	113.75	110.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

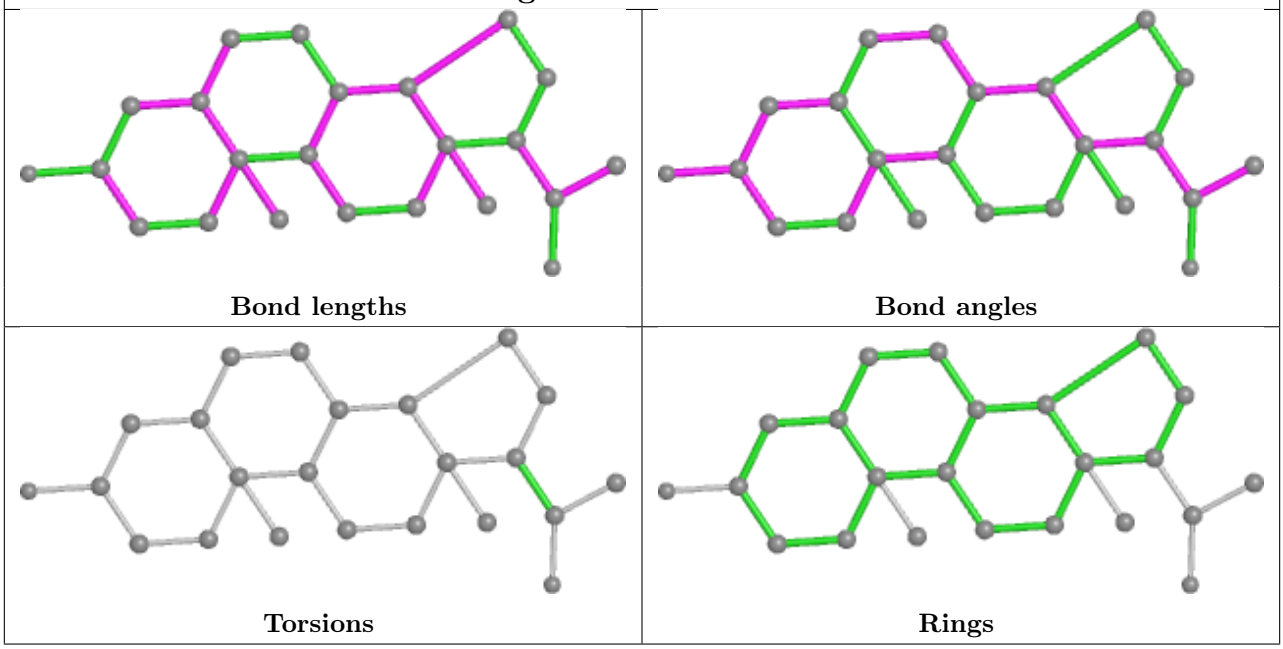
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	STR	2	0
2	A	1001	STR	1	0
2	C	3001	STR	12	0

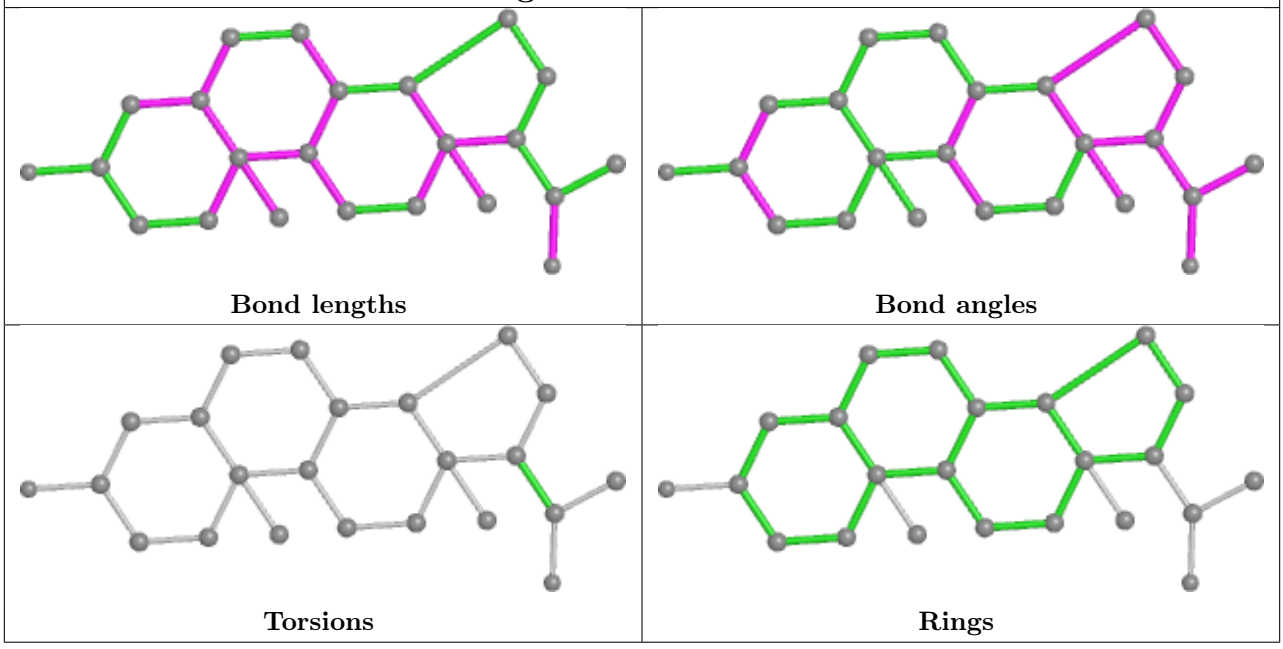
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

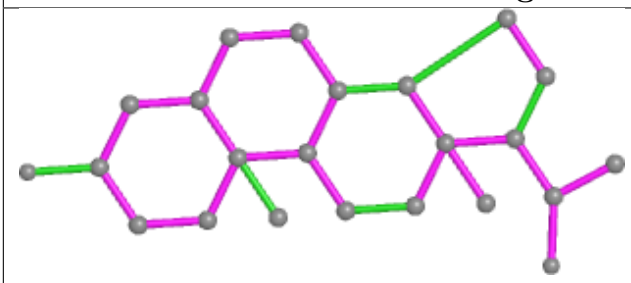
Ligand STR B 2001



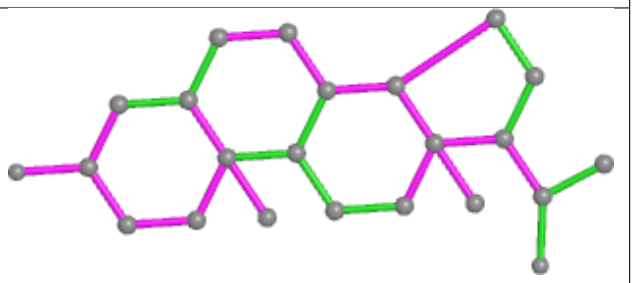
Ligand STR A 1001



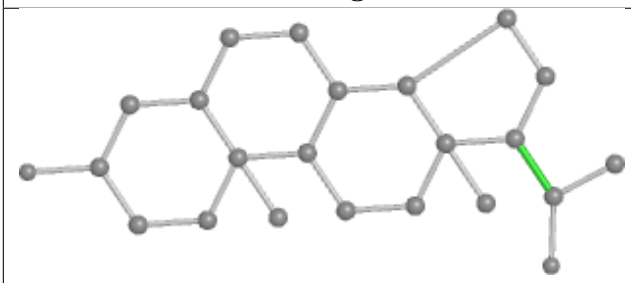
Ligand STR C 3001



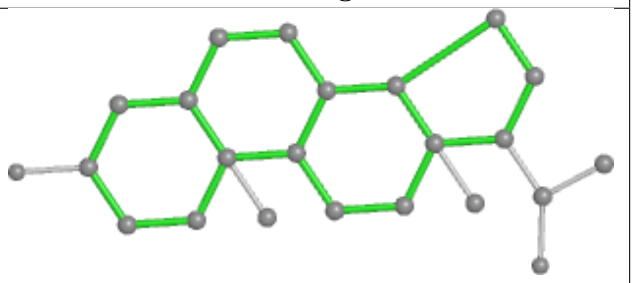
Bond lengths



Bond angles



Torsions



Rings

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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	973:SER	C	974:GLY	N	1.04

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	233/255 (91%)	0.31	14 (6%)	21	30	25, 45, 67, 75	0
1	B	230/255 (90%)	0.27	9 (3%)	39	50	32, 50, 66, 71	0
1	C	232/255 (90%)	0.25	9 (3%)	39	50	30, 50, 64, 73	0
All	All	695/765 (90%)	0.28	32 (4%)	32	43	25, 48, 66, 75	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	749	ILE	4.1
1	C	950	HIS	3.9
1	B	950	HIS	3.8
1	C	908	THR	3.6
1	C	952	LEU	3.5
1	B	749	ILE	3.3
1	A	973	SER	3.2
1	A	908	THR	3.2
1	B	752	ALA	3.2
1	A	753	GLY	3.1
1	A	754	TYR	3.1
1	A	951	ALA	2.9
1	C	974	GLY	2.8
1	C	951	ALA	2.7
1	A	838	GLU	2.7
1	B	838	GLU	2.6
1	A	820	LYS	2.6
1	A	821	HIS	2.6
1	C	756	SER	2.5
1	A	760	ASP	2.5
1	B	951	ALA	2.5
1	A	846	TYR	2.4
1	B	821	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	760	ASP	2.4
1	A	969	PRO	2.4
1	C	837	GLU	2.3
1	B	974	GLY	2.2
1	B	843	SER	2.2
1	A	752	ALA	2.1
1	A	837	GLU	2.1
1	C	859	PHE	2.1
1	C	755	ASP	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)

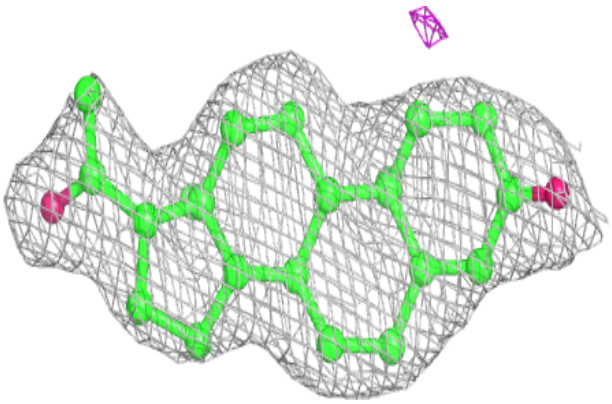
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

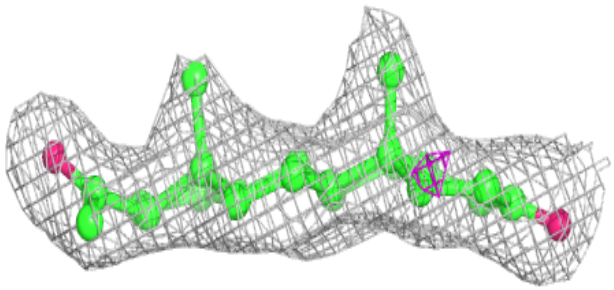
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	STR	C	3001	23/23	0.90	0.20	37,40,42,45	0
2	STR	B	2001	23/23	0.94	0.27	36,37,43,47	0
2	STR	A	1001	23/23	0.94	0.21	30,32,34,36	0

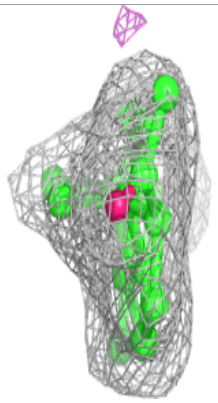
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around STR C 3001:

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

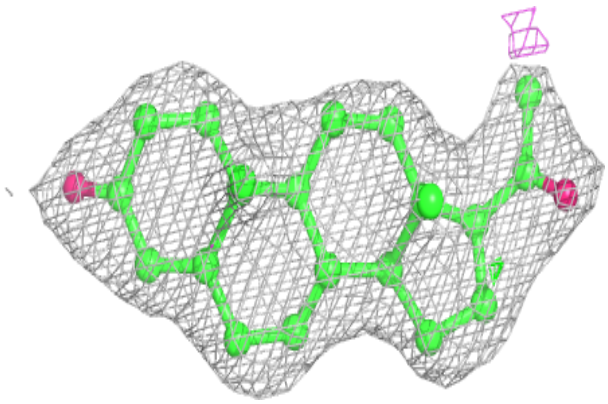


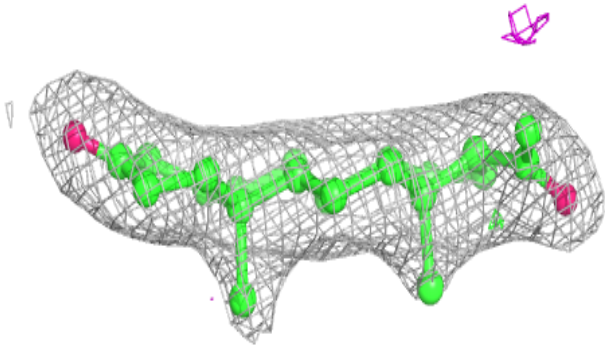


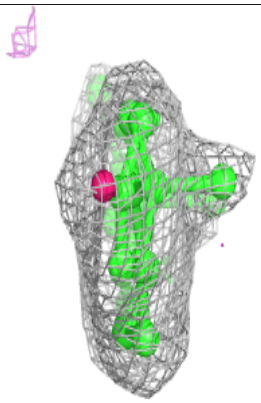


Electron density around STR B 2001:

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

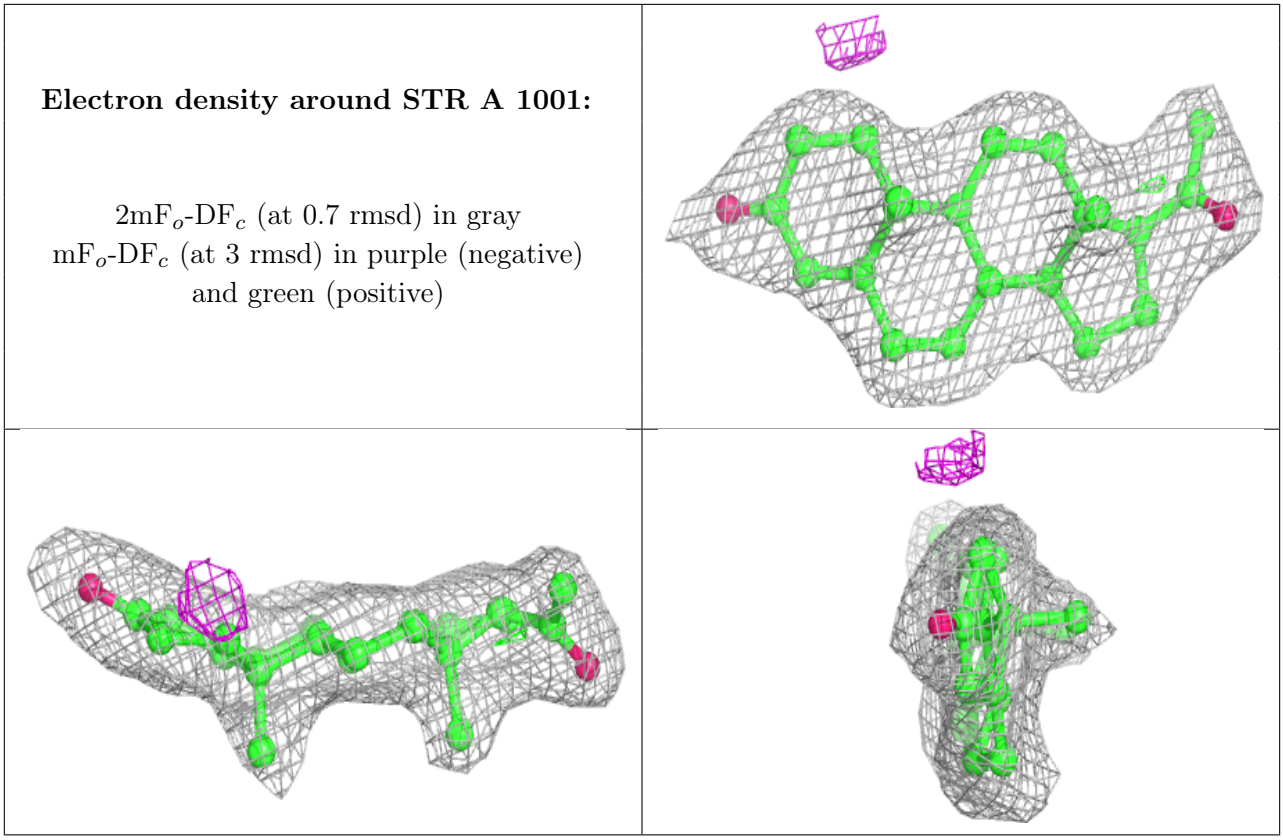






Electron density around STR A 1001:

$2mF_o$-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.