



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:44 AM BST

PDB ID : 6VKQ
Title : Crystal Structure of human PARP-1 CAT domain bound to inhibitor EB-47
Authors : Steffen, J.D.; Pascal, J.M.
Deposited on : 2020-01-21
Resolution : 2.90 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 : 2.13.1
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) : 2.13.1

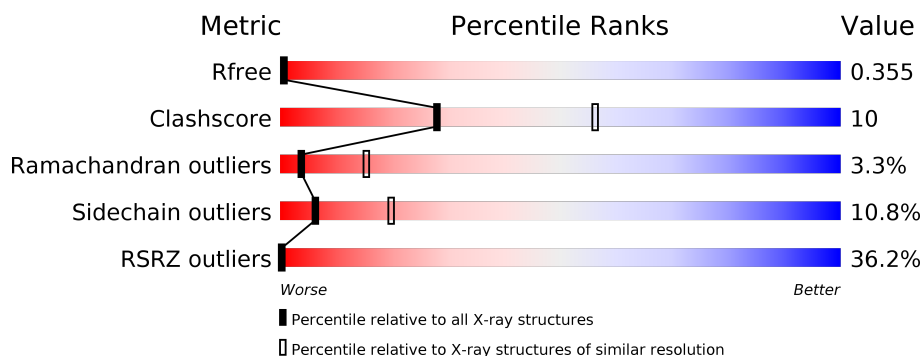
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	<div> <div>33%</div> <div> <div>63%</div> <div>24%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	372	<div> <div>36%</div> <div> <div>66%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	372	<div> <div>32%</div> <div> <div>64%</div> <div>23%</div> <div>•</div> <div>9%</div> </div> </div>
1	D	372	<div> <div>32%</div> <div> <div>65%</div> <div>22%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10910 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2678	1709	453	505	11			
1	B	340	Total	C	N	O	S	0	0	0
			2672	1706	450	505	11			
1	C	340	Total	C	N	O	S	0	0	0
			2672	1706	450	505	11			
1	D	340	Total	C	N	O	S	0	0	0
			2672	1706	450	505	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	MET	-	initiating methionine	UNP P09874
A	641	GLY	-	expression tag	UNP P09874
A	642	SER	-	expression tag	UNP P09874
A	643	SER	-	expression tag	UNP P09874
A	644	HIS	-	expression tag	UNP P09874
A	645	HIS	-	expression tag	UNP P09874
A	646	HIS	-	expression tag	UNP P09874
A	647	HIS	-	expression tag	UNP P09874
A	648	HIS	-	expression tag	UNP P09874
A	649	HIS	-	expression tag	UNP P09874
A	650	SER	-	expression tag	UNP P09874
A	651	SER	-	expression tag	UNP P09874
A	652	GLY	-	expression tag	UNP P09874
A	653	LEU	-	expression tag	UNP P09874
A	654	VAL	-	expression tag	UNP P09874
A	655	PRO	-	expression tag	UNP P09874
A	656	ARG	-	expression tag	UNP P09874
A	657	GLY	-	expression tag	UNP P09874
A	658	SER	-	expression tag	UNP P09874
A	659	HIS	-	expression tag	UNP P09874
A	660	MET	-	expression tag	UNP P09874

Continued on next page...

Continued from previous page...

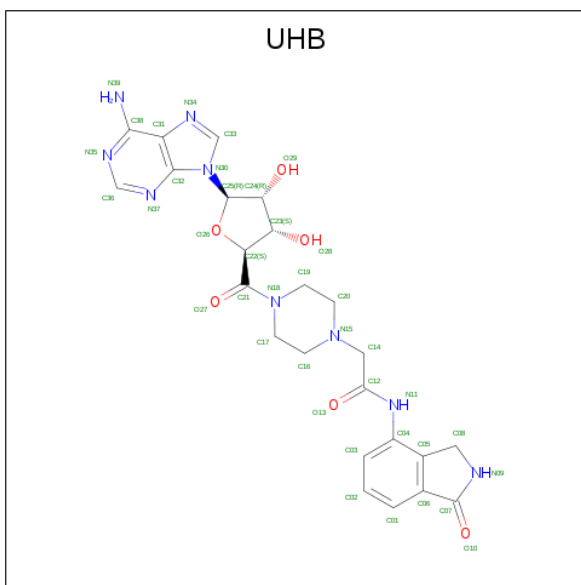
Chain	Residue	Modelled	Actual	Comment	Reference
A	762	ALA	VAL	variant	UNP P09874
B	640	MET	-	initiating methionine	UNP P09874
B	641	GLY	-	expression tag	UNP P09874
B	642	SER	-	expression tag	UNP P09874
B	643	SER	-	expression tag	UNP P09874
B	644	HIS	-	expression tag	UNP P09874
B	645	HIS	-	expression tag	UNP P09874
B	646	HIS	-	expression tag	UNP P09874
B	647	HIS	-	expression tag	UNP P09874
B	648	HIS	-	expression tag	UNP P09874
B	649	HIS	-	expression tag	UNP P09874
B	650	SER	-	expression tag	UNP P09874
B	651	SER	-	expression tag	UNP P09874
B	652	GLY	-	expression tag	UNP P09874
B	653	LEU	-	expression tag	UNP P09874
B	654	VAL	-	expression tag	UNP P09874
B	655	PRO	-	expression tag	UNP P09874
B	656	ARG	-	expression tag	UNP P09874
B	657	GLY	-	expression tag	UNP P09874
B	658	SER	-	expression tag	UNP P09874
B	659	HIS	-	expression tag	UNP P09874
B	660	MET	-	expression tag	UNP P09874
B	762	ALA	VAL	variant	UNP P09874
C	640	MET	-	initiating methionine	UNP P09874
C	641	GLY	-	expression tag	UNP P09874
C	642	SER	-	expression tag	UNP P09874
C	643	SER	-	expression tag	UNP P09874
C	644	HIS	-	expression tag	UNP P09874
C	645	HIS	-	expression tag	UNP P09874
C	646	HIS	-	expression tag	UNP P09874
C	647	HIS	-	expression tag	UNP P09874
C	648	HIS	-	expression tag	UNP P09874
C	649	HIS	-	expression tag	UNP P09874
C	650	SER	-	expression tag	UNP P09874
C	651	SER	-	expression tag	UNP P09874
C	652	GLY	-	expression tag	UNP P09874
C	653	LEU	-	expression tag	UNP P09874
C	654	VAL	-	expression tag	UNP P09874
C	655	PRO	-	expression tag	UNP P09874
C	656	ARG	-	expression tag	UNP P09874
C	657	GLY	-	expression tag	UNP P09874
C	658	SER	-	expression tag	UNP P09874

Continued on next page...

Continued from previous page...

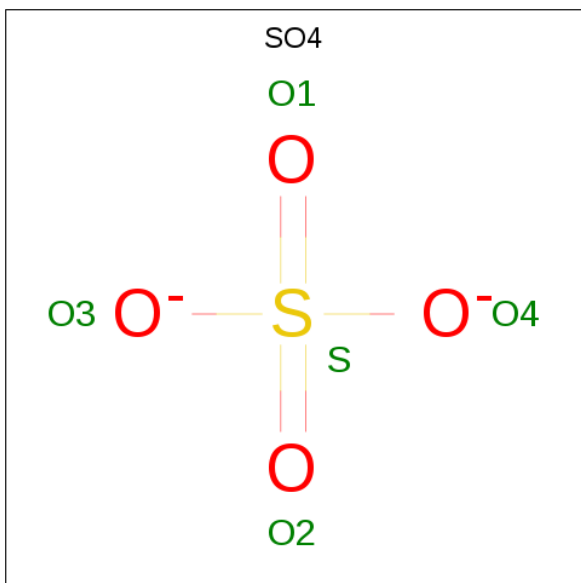
Chain	Residue	Modelled	Actual	Comment	Reference
C	659	HIS	-	expression tag	UNP P09874
C	660	MET	-	expression tag	UNP P09874
C	762	ALA	VAL	variant	UNP P09874
D	640	MET	-	initiating methionine	UNP P09874
D	641	GLY	-	expression tag	UNP P09874
D	642	SER	-	expression tag	UNP P09874
D	643	SER	-	expression tag	UNP P09874
D	644	HIS	-	expression tag	UNP P09874
D	645	HIS	-	expression tag	UNP P09874
D	646	HIS	-	expression tag	UNP P09874
D	647	HIS	-	expression tag	UNP P09874
D	648	HIS	-	expression tag	UNP P09874
D	649	HIS	-	expression tag	UNP P09874
D	650	SER	-	expression tag	UNP P09874
D	651	SER	-	expression tag	UNP P09874
D	652	GLY	-	expression tag	UNP P09874
D	653	LEU	-	expression tag	UNP P09874
D	654	VAL	-	expression tag	UNP P09874
D	655	PRO	-	expression tag	UNP P09874
D	656	ARG	-	expression tag	UNP P09874
D	657	GLY	-	expression tag	UNP P09874
D	658	SER	-	expression tag	UNP P09874
D	659	HIS	-	expression tag	UNP P09874
D	660	MET	-	expression tag	UNP P09874
D	762	ALA	VAL	variant	UNP P09874

- Molecule 2 is 2-[4-[(2S,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]carbon ylpiperazin-1-yl]-N-(1-oxidanylidene-2,3-dihydroisindol-4-yl)ethanamide (three-letter code: UHB) (formula: C₂₄H₂₇N₉O₆) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			39	24	9	6		
2	B	1	Total	C	N	O	0	0
			39	24	9	6		
2	C	1	Total	C	N	O	0	0
			39	24	9	6		
2	D	1	Total	C	N	O	0	0
			39	24	9	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).

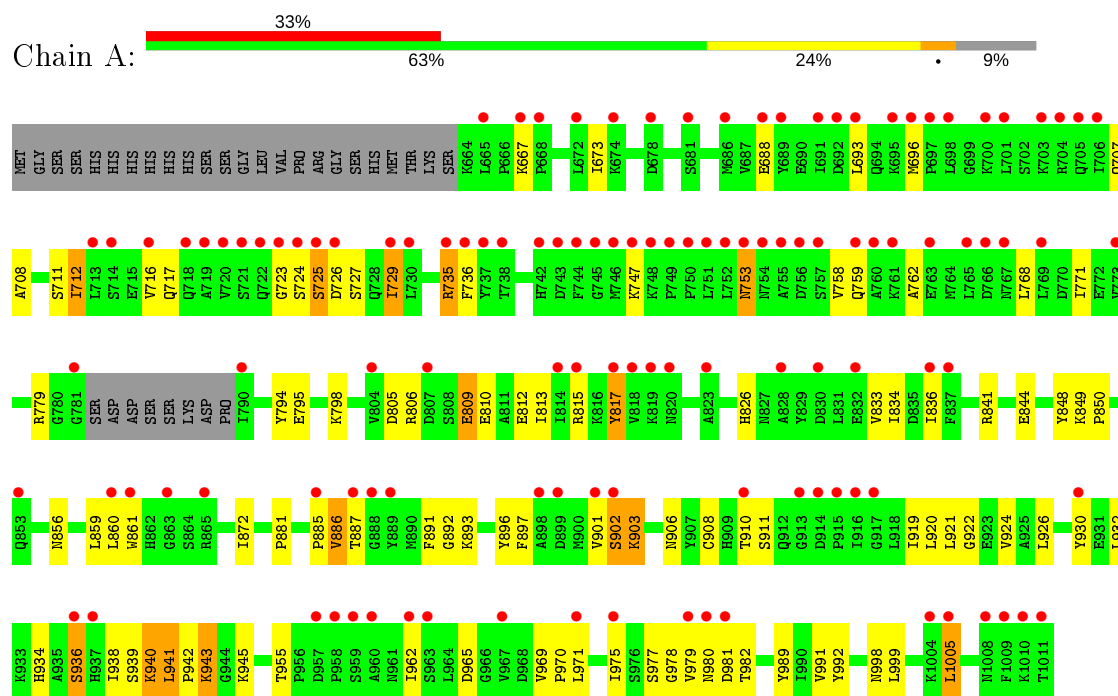


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

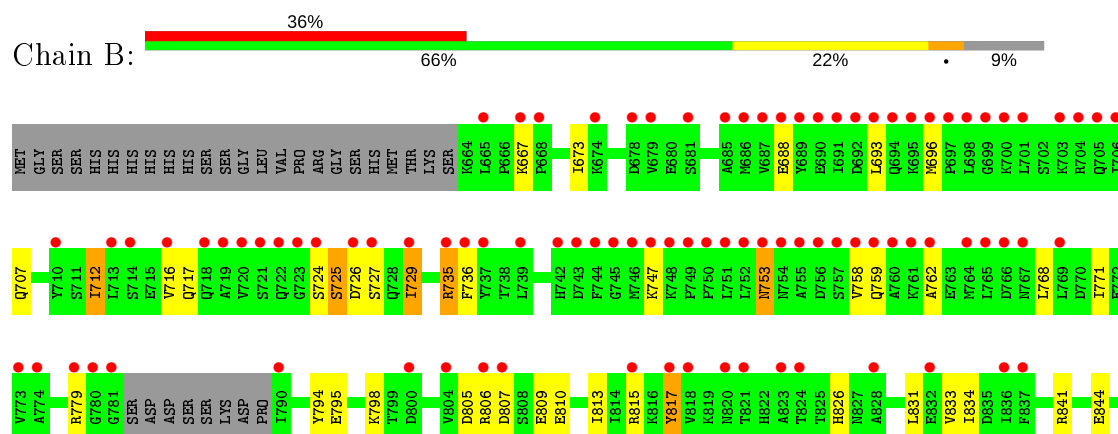
3 Residue-property plots

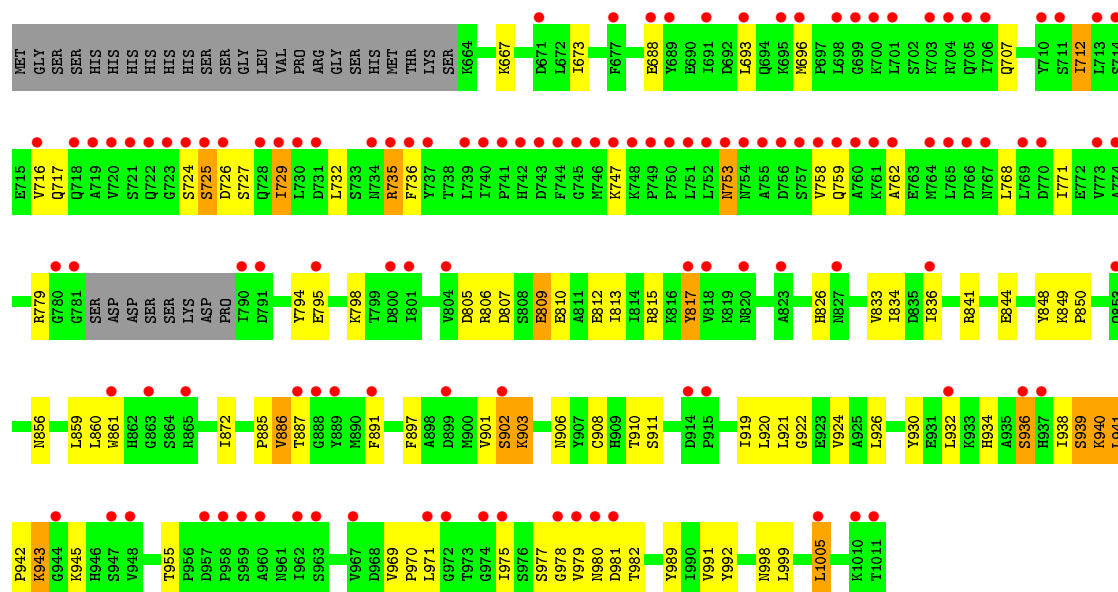
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Poly [ADP-ribose] polymerase 1



- Molecule 1: Poly [ADP-ribose] polymerase 1





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.22Å 130.31Å 101.87Å 90.00° 111.25° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 47.47 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.90) 99.3 (47.47-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.91Å)	Xtrriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.323 , 0.353 0.327 , 0.355	Depositor DCC
R_{free} test set	1909 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtrriage
Anisotropy	0.433	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10910	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.45 % 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 $7.0655e-06$. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UHB, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	0/2728	0.79	0/3681
1	B	0.69	0/2722	0.79	0/3674
1	C	0.69	0/2722	0.80	0/3674
1	D	0.69	0/2722	0.80	0/3674
All	All	0.69	0/10894	0.79	0/14703

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 [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	2678	0	2725	58	0
1	B	2672	0	2714	55	0
1	C	2672	0	2714	58	0
1	D	2672	0	2714	54	0
2	A	39	0	27	1	0
2	B	39	0	27	0	0
2	C	39	0	27	1	0
2	D	39	0	27	0	0
3	A	15	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	1	0
3	C	15	0	0	0	0
3	D	15	0	0	0	0
All	All	10910	0	10975	217	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 10.

All (217) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:962:ILE:HG23	1:C:939:SER:HB2	1.59	0.82
1:C:962:ILE:HG23	1:D:939:SER:HB2	1.58	0.81
1:A:962:ILE:HG23	1:B:939:SER:HB2	1.64	0.79
1:C:977:SER:O	1:C:979:VAL:N	2.17	0.78
1:B:977:SER:O	1:B:979:VAL:N	2.17	0.77
1:A:977:SER:O	1:A:979:VAL:N	2.17	0.76
1:D:977:SER:O	1:D:979:VAL:N	2.16	0.76
1:B:859:LEU:HA	1:B:922:GLY:O	1.86	0.76
1:D:859:LEU:HA	1:D:922:GLY:O	1.86	0.76
1:C:859:LEU:HA	1:C:922:GLY:O	1.86	0.75
1:A:859:LEU:HA	1:A:922:GLY:O	1.86	0.73
1:D:891:PHE:HA	1:D:936:SER:O	1.95	0.67
1:A:891:PHE:HA	1:A:936:SER:O	1.95	0.67
1:B:891:PHE:HA	1:B:936:SER:O	1.94	0.67
1:C:891:PHE:HA	1:C:936:SER:O	1.94	0.66
1:D:860:LEU:HD12	1:D:924:VAL:CG2	2.30	0.62
1:A:860:LEU:HD12	1:A:924:VAL:CG2	2.30	0.62
1:A:941:LEU:HD21	1:A:992:TYR:CD1	2.35	0.61
1:B:860:LEU:HD12	1:B:924:VAL:CG2	2.30	0.61
1:C:941:LEU:HD21	1:C:992:TYR:CD1	2.35	0.61
1:D:941:LEU:HD21	1:D:992:TYR:CD1	2.36	0.61
1:C:860:LEU:HD12	1:C:924:VAL:CG2	2.31	0.61
1:D:897:PHE:CE1	1:D:924:VAL:HG11	2.35	0.61
1:A:897:PHE:CE1	1:A:924:VAL:HG11	2.36	0.60
1:B:897:PHE:CE1	1:B:924:VAL:HG11	2.35	0.60
1:B:941:LEU:HD21	1:B:992:TYR:CD1	2.36	0.60
1:C:897:PHE:CE1	1:C:924:VAL:HG11	2.36	0.60
1:D:859:LEU:CD2	1:D:921:LEU:HD22	2.32	0.60
1:C:859:LEU:CD2	1:C:921:LEU:HD22	2.32	0.59
1:A:859:LEU:CD2	1:A:921:LEU:HD22	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:859:LEU:CD2	1:B:921:LEU:HD22	2.32	0.59
1:C:762:ALA:HB2	1:C:885:PRO:HG2	1.85	0.59
1:B:941:LEU:HD21	1:B:992:TYR:HD1	1.67	0.58
1:D:762:ALA:HB2	1:D:885:PRO:HG2	1.85	0.58
1:C:932:LEU:HD13	1:C:936:SER:OG	2.04	0.58
1:C:941:LEU:HD21	1:C:992:TYR:HD1	1.68	0.58
1:D:932:LEU:HD13	1:D:936:SER:OG	2.04	0.58
1:D:941:LEU:HD21	1:D:992:TYR:HD1	1.68	0.58
1:B:932:LEU:HD13	1:B:936:SER:OG	2.04	0.58
1:D:977:SER:C	1:D:979:VAL:H	2.07	0.58
1:B:977:SER:C	1:B:979:VAL:H	2.07	0.57
1:A:977:SER:C	1:A:979:VAL:H	2.07	0.57
1:A:932:LEU:HD13	1:A:936:SER:OG	2.04	0.57
1:A:762:ALA:HB2	1:A:885:PRO:HG2	1.88	0.56
1:A:941:LEU:HD21	1:A:992:TYR:HD1	1.68	0.56
1:B:969:VAL:HG12	1:B:971:LEU:HD23	1.87	0.56
1:C:977:SER:C	1:C:979:VAL:H	2.07	0.56
1:D:969:VAL:HG12	1:D:971:LEU:HD23	1.87	0.56
1:B:762:ALA:HB2	1:B:885:PRO:HG2	1.87	0.56
1:C:969:VAL:HG12	1:C:971:LEU:HD23	1.88	0.56
1:B:844:GLU:HG2	1:B:998:ASN:HD22	1.72	0.55
1:A:969:VAL:HG12	1:A:971:LEU:HD23	1.86	0.55
1:C:844:GLU:HG2	1:C:998:ASN:HD22	1.71	0.55
1:A:844:GLU:HG2	1:A:998:ASN:HD22	1.71	0.54
1:D:844:GLU:HG2	1:D:998:ASN:HD22	1.72	0.53
1:B:859:LEU:HD23	1:B:921:LEU:HD22	1.91	0.53
1:A:980:ASN:O	1:A:982:THR:N	2.35	0.53
1:C:962:ILE:CG2	1:D:939:SER:HB2	2.35	0.53
1:C:859:LEU:HD23	1:C:921:LEU:HD22	1.91	0.53
1:A:841:ARG:HD3	1:A:999:LEU:HD12	1.92	0.52
1:C:841:ARG:HD3	1:C:999:LEU:HD12	1.92	0.52
1:C:980:ASN:O	1:C:982:THR:N	2.35	0.52
1:A:892:GLY:O	1:A:896:TYR:OH	2.19	0.52
1:D:859:LEU:HD23	1:D:921:LEU:HD22	1.90	0.52
1:D:841:ARG:HD3	1:D:999:LEU:HD12	1.92	0.51
1:A:859:LEU:HD23	1:A:921:LEU:HD22	1.91	0.51
1:A:861:TRP:CD2	1:A:901:VAL:HG23	2.46	0.51
1:B:969:VAL:CG1	1:B:971:LEU:HD23	2.41	0.51
1:B:861:TRP:CD2	1:B:901:VAL:HG23	2.46	0.51
1:D:977:SER:OG	1:D:977:SER:O	2.29	0.51
1:D:753:ASN:HD22	1:D:753:ASN:H	1.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:980:ASN:C	1:D:982:THR:H	2.15	0.50
1:A:969:VAL:CG1	1:A:971:LEU:HD23	2.41	0.50
1:B:753:ASN:HD22	1:B:753:ASN:H	1.59	0.50
1:C:861:TRP:CD2	1:C:901:VAL:HG23	2.46	0.50
1:D:861:TRP:CD2	1:D:901:VAL:HG23	2.46	0.50
1:B:841:ARG:HD3	1:B:999:LEU:HD12	1.93	0.50
1:C:892:GLY:O	1:C:896:TYR:OH	2.18	0.50
1:A:860:LEU:HD12	1:A:924:VAL:HG21	1.94	0.49
1:C:753:ASN:H	1:C:753:ASN:HD22	1.59	0.49
1:D:980:ASN:O	1:D:982:THR:N	2.35	0.49
1:A:768:LEU:HA	1:A:771:ILE:HB	1.95	0.49
1:A:753:ASN:HD22	1:A:753:ASN:H	1.59	0.49
1:B:768:LEU:HA	1:B:771:ILE:HB	1.95	0.49
1:B:980:ASN:C	1:B:982:THR:H	2.15	0.49
1:C:969:VAL:CG1	1:C:971:LEU:HD23	2.43	0.49
1:D:826:HIS:ND1	1:D:902:SER:HB2	2.28	0.49
1:A:980:ASN:C	1:A:982:THR:H	2.15	0.48
1:B:826:HIS:ND1	1:B:902:SER:HB2	2.28	0.48
1:C:826:HIS:ND1	1:C:902:SER:HB2	2.29	0.48
1:B:980:ASN:O	1:B:982:THR:N	2.36	0.48
1:D:768:LEU:HA	1:D:771:ILE:HB	1.95	0.48
1:C:768:LEU:HA	1:C:771:ILE:HB	1.95	0.48
1:C:817:TYR:CE1	1:C:970:PRO:O	2.67	0.48
1:B:817:TYR:CE1	1:B:970:PRO:O	2.67	0.48
1:C:980:ASN:C	1:C:982:THR:H	2.15	0.48
1:D:860:LEU:HD12	1:D:924:VAL:HG21	1.96	0.48
1:D:969:VAL:CG1	1:D:971:LEU:HD23	2.43	0.48
1:A:712:ILE:HD12	1:A:735:ARG:HD2	1.96	0.47
1:A:826:HIS:ND1	1:A:902:SER:HB2	2.29	0.47
1:C:712:ILE:HD12	1:C:735:ARG:HD2	1.96	0.47
1:A:817:TYR:CE1	1:A:970:PRO:O	2.67	0.47
1:D:919:ILE:HG21	1:D:1005:LEU:HD21	1.97	0.47
1:D:817:TYR:CE1	1:D:970:PRO:O	2.67	0.47
1:A:848:TYR:CG	1:A:998:ASN:HB2	2.50	0.46
1:B:848:TYR:CG	1:B:998:ASN:HB2	2.50	0.46
1:A:919:ILE:HG21	1:A:1005:LEU:HD21	1.97	0.46
1:C:860:LEU:HD12	1:C:924:VAL:HG21	1.96	0.46
1:B:942:PRO:O	1:B:943:LYS:O	2.34	0.46
1:C:942:PRO:O	1:C:943:LYS:O	2.34	0.46
1:D:848:TYR:CG	1:D:998:ASN:HB2	2.51	0.46
1:A:930:TYR:CZ	1:A:932:LEU:HD21	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:813:ILE:HD13	1:C:813:ILE:N	2.31	0.46
1:C:712:ILE:HG21	1:C:736:PHE:HB2	1.98	0.45
1:D:942:PRO:O	1:D:943:LYS:O	2.34	0.45
1:A:813:ILE:N	1:A:813:ILE:HD13	2.31	0.45
1:B:860:LEU:HD12	1:B:924:VAL:HG21	1.96	0.45
1:D:849:LYS:HB3	1:D:850:PRO:HD3	1.98	0.45
1:D:930:TYR:CZ	1:D:932:LEU:HD21	2.51	0.45
1:D:955:THR:O	1:D:975:ILE:HG22	2.17	0.45
1:B:813:ILE:N	1:B:813:ILE:HD13	2.31	0.45
1:B:930:TYR:CZ	1:B:932:LEU:HD21	2.52	0.45
1:B:725:SER:C	1:B:729:ILE:HG13	2.37	0.45
1:C:919:ILE:HG21	1:C:1005:LEU:HD21	1.98	0.45
1:B:965:ASP:HA	1:C:942:PRO:HA	1.97	0.45
1:D:897:PHE:N	1:D:989:TYR:O	2.36	0.45
1:B:712:ILE:HG21	1:B:736:PHE:HB2	1.98	0.45
1:C:848:TYR:CG	1:C:998:ASN:HB2	2.51	0.45
1:D:725:SER:C	1:D:729:ILE:HG13	2.37	0.45
1:D:712:ILE:HD12	1:D:735:ARG:HD2	1.98	0.45
1:A:725:SER:C	1:A:729:ILE:HG13	2.37	0.45
1:A:942:PRO:O	1:A:943:LYS:O	2.34	0.45
1:B:919:ILE:CG2	1:B:1005:LEU:HD21	2.47	0.45
1:C:872:ILE:HG21	1:C:920:LEU:HD11	1.99	0.45
1:D:712:ILE:HG21	1:D:736:PHE:HB2	1.98	0.45
1:B:919:ILE:HG21	1:B:1005:LEU:HD21	1.97	0.45
1:C:955:THR:O	1:C:975:ILE:HG22	2.17	0.45
1:A:955:THR:O	1:A:975:ILE:HG22	2.17	0.45
1:C:856:ASN:ND2	1:C:926:LEU:HB2	2.32	0.45
1:D:813:ILE:HD13	1:D:813:ILE:N	2.31	0.45
1:C:725:SER:C	1:C:729:ILE:HG13	2.37	0.45
1:A:712:ILE:HG21	1:A:736:PHE:HB2	1.98	0.44
1:A:872:ILE:HG21	1:A:920:LEU:HD11	1.99	0.44
1:B:806:ARG:O	1:B:815:ARG:NH2	2.50	0.44
1:A:897:PHE:N	1:A:989:TYR:O	2.35	0.44
1:D:908:CYS:HB3	1:D:910:THR:HG23	1.99	0.44
1:B:856:ASN:ND2	1:B:926:LEU:HB2	2.33	0.44
1:B:955:THR:O	1:B:975:ILE:HG22	2.17	0.44
1:C:759:GLN:O	1:C:762:ALA:HB3	2.18	0.44
1:C:908:CYS:HB3	1:C:910:THR:HG23	2.00	0.44
2:A:2001:UHB:H20	2:A:2001:UHB:O13	2.17	0.44
1:A:759:GLN:O	1:A:762:ALA:HB3	2.17	0.44
1:B:897:PHE:HB2	1:B:989:TYR:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:ARG:CB	2:C:2001:UHB:N39	2.81	0.44
1:D:759:GLN:O	1:D:762:ALA:HB3	2.18	0.44
1:D:872:ILE:HG21	1:D:920:LEU:HD11	1.99	0.44
1:C:930:TYR:CZ	1:C:932:LEU:HD21	2.52	0.44
1:D:806:ARG:O	1:D:815:ARG:NH2	2.50	0.44
1:A:897:PHE:HB2	1:A:989:TYR:HB2	2.00	0.44
1:B:759:GLN:O	1:B:762:ALA:HB3	2.18	0.44
1:B:897:PHE:N	1:B:989:TYR:O	2.36	0.43
1:D:919:ILE:CG2	1:D:1005:LEU:HD21	2.48	0.43
1:A:908:CYS:HB3	1:A:910:THR:HG23	2.00	0.43
1:D:856:ASN:ND2	1:D:926:LEU:HB2	2.32	0.43
1:A:856:ASN:ND2	1:A:926:LEU:HB2	2.33	0.43
1:A:919:ILE:CG2	1:A:1005:LEU:HD21	2.47	0.43
1:B:872:ILE:HG21	1:B:920:LEU:HD11	1.99	0.43
1:B:962:ILE:CG2	1:C:939:SER:HB2	2.39	0.43
1:A:806:ARG:O	1:A:815:ARG:NH2	2.50	0.43
1:B:903:LYS:HA	1:B:906:ASN:HD22	1.84	0.43
1:C:897:PHE:CZ	1:C:924:VAL:HG11	2.53	0.43
1:D:897:PHE:CZ	1:D:924:VAL:HG11	2.53	0.43
1:B:712:ILE:HD12	1:B:735:ARG:HD2	1.99	0.43
1:C:849:LYS:HB3	1:C:850:PRO:HD3	2.01	0.43
1:C:897:PHE:HB2	1:C:989:TYR:HB2	2.00	0.43
1:D:903:LYS:HA	1:D:906:ASN:HD22	1.83	0.43
1:B:858:ARG:NH2	3:B:2003:SO4:O4	2.52	0.43
1:A:965:ASP:HA	1:B:942:PRO:HA	2.00	0.43
1:A:903:LYS:HA	1:A:906:ASN:HD22	1.84	0.43
1:C:919:ILE:CG2	1:C:1005:LEU:HD21	2.49	0.43
1:C:903:LYS:HA	1:C:906:ASN:HD22	1.84	0.42
1:D:897:PHE:HB2	1:D:989:TYR:HB2	2.00	0.42
1:A:725:SER:O	1:A:727:SER:N	2.53	0.42
1:B:725:SER:O	1:B:727:SER:N	2.53	0.42
1:D:673:ILE:HD13	1:D:794:TYR:HB2	2.02	0.42
1:B:897:PHE:CZ	1:B:924:VAL:HG11	2.54	0.42
1:C:806:ARG:O	1:C:815:ARG:NH2	2.51	0.42
1:B:908:CYS:HB3	1:B:910:THR:HG23	2.01	0.42
1:A:673:ILE:HD13	1:A:794:TYR:HB2	2.02	0.42
1:A:809:GLU:O	1:A:812:GLU:N	2.50	0.42
1:C:725:SER:O	1:C:727:SER:N	2.53	0.42
1:C:965:ASP:HA	1:D:942:PRO:HA	2.02	0.41
1:B:717:GLN:OE1	1:B:758:VAL:HG11	2.20	0.41
1:C:673:ILE:HD13	1:C:794:TYR:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:GLN:OE1	1:A:758:VAL:HG11	2.20	0.41
1:D:725:SER:O	1:D:727:SER:N	2.53	0.41
1:B:831:LEU:HA	1:B:831:LEU:HD12	1.92	0.41
1:B:977:SER:OG	1:B:977:SER:O	2.29	0.41
1:A:849:LYS:NZ	3:A:2004:SO4:O4	2.49	0.41
1:A:977:SER:C	1:A:979:VAL:N	2.72	0.41
1:D:717:GLN:OE1	1:D:758:VAL:HG11	2.20	0.41
1:B:673:ILE:HD13	1:B:794:TYR:HB2	2.02	0.41
1:D:930:TYR:CE1	1:D:932:LEU:HD21	2.56	0.41
1:A:708:ALA:O	1:A:711:SER:OG	2.27	0.41
1:C:717:GLN:OE1	1:C:758:VAL:HG11	2.20	0.41
1:C:725:SER:H	1:C:729:ILE:HD11	1.86	0.41
1:C:886:VAL:HG23	1:C:887:THR:H	1.86	0.41
1:A:725:SER:H	1:A:729:ILE:HD11	1.87	0.40
1:A:849:LYS:HB3	1:A:850:PRO:HD3	2.01	0.40
1:A:962:ILE:CG2	1:B:939:SER:HB2	2.43	0.40
1:C:831:LEU:HA	1:C:831:LEU:HD12	1.93	0.40
1:A:897:PHE:CZ	1:A:924:VAL:HG11	2.55	0.40
1:D:729:ILE:O	1:D:732:LEU:N	2.55	0.40
1:D:809:GLU:O	1:D:812:GLU:N	2.50	0.40
1:A:881:PRO:O	1:A:893:LYS:NZ	2.42	0.40
1:A:924:VAL:O	1:A:924:VAL:HG23	2.22	0.40
1:C:719:ALA:HB1	1:C:724:SER:HB3	2.04	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	336/372 (90%)	288 (86%)	36 (11%)	12 (4%)	3	14
1	B	336/372 (90%)	287 (85%)	38 (11%)	11 (3%)	4	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	336/372 (90%)	288 (86%)	37 (11%)	11 (3%)	4	15
1	D	336/372 (90%)	287 (85%)	38 (11%)	11 (3%)	4	15
All	All	1344/1488 (90%)	1150 (86%)	149 (11%)	45 (3%)	4	15

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	886	VAL
1	A	940	LYS
1	A	943	LYS
1	A	978	GLY
1	A	981	ASP
1	B	886	VAL
1	B	940	LYS
1	B	943	LYS
1	B	978	GLY
1	B	981	ASP
1	C	886	VAL
1	C	940	LYS
1	C	943	LYS
1	C	978	GLY
1	C	981	ASP
1	D	886	VAL
1	D	940	LYS
1	D	943	LYS
1	D	978	GLY
1	D	981	ASP
1	A	716	VAL
1	B	716	VAL
1	C	716	VAL
1	D	716	VAL
1	A	726	ASP
1	A	810	GLU
1	B	726	ASP
1	B	810	GLU
1	C	726	ASP
1	C	810	GLU
1	D	725	SER
1	D	726	ASP
1	D	810	GLU
1	A	725	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	798	LYS
1	B	725	SER
1	B	798	LYS
1	C	725	SER
1	C	798	LYS
1	D	798	LYS
1	A	834	ILE
1	C	834	ILE
1	D	834	ILE
1	B	834	ILE
1	A	723	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/326 (91%)	265 (89%)	32 (11%)	6	20
1	B	296/326 (91%)	265 (90%)	31 (10%)	7	21
1	C	296/326 (91%)	264 (89%)	32 (11%)	6	20
1	D	296/326 (91%)	263 (89%)	33 (11%)	6	19
All	All	1185/1304 (91%)	1057 (89%)	128 (11%)	6	20

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	667	LYS
1	A	688	GLU
1	A	693	LEU
1	A	696	MET
1	A	707	GLN
1	A	712	ILE
1	A	724	SER
1	A	729	ILE
1	A	735	ARG
1	A	747	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	753	ASN
1	A	779	ARG
1	A	795	GLU
1	A	805	ASP
1	A	809	GLU
1	A	817	TYR
1	A	833	VAL
1	A	836	ILE
1	A	886	VAL
1	A	887	THR
1	A	902	SER
1	A	903	LYS
1	A	911	SER
1	A	934	HIS
1	A	936	SER
1	A	938	ILE
1	A	939	SER
1	A	940	LYS
1	A	941	LEU
1	A	945	LYS
1	A	991	VAL
1	A	1005	LEU
1	B	667	LYS
1	B	688	GLU
1	B	693	LEU
1	B	696	MET
1	B	707	GLN
1	B	712	ILE
1	B	724	SER
1	B	729	ILE
1	B	735	ARG
1	B	747	LYS
1	B	753	ASN
1	B	779	ARG
1	B	795	GLU
1	B	805	ASP
1	B	807	ASP
1	B	809	GLU
1	B	817	TYR
1	B	833	VAL
1	B	886	VAL
1	B	887	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	902	SER
1	B	903	LYS
1	B	911	SER
1	B	934	HIS
1	B	936	SER
1	B	938	ILE
1	B	939	SER
1	B	941	LEU
1	B	945	LYS
1	B	991	VAL
1	B	1005	LEU
1	C	667	LYS
1	C	688	GLU
1	C	693	LEU
1	C	696	MET
1	C	707	GLN
1	C	712	ILE
1	C	724	SER
1	C	729	ILE
1	C	735	ARG
1	C	747	LYS
1	C	753	ASN
1	C	779	ARG
1	C	795	GLU
1	C	805	ASP
1	C	807	ASP
1	C	809	GLU
1	C	817	TYR
1	C	833	VAL
1	C	836	ILE
1	C	886	VAL
1	C	887	THR
1	C	902	SER
1	C	903	LYS
1	C	911	SER
1	C	934	HIS
1	C	936	SER
1	C	938	ILE
1	C	939	SER
1	C	940	LYS
1	C	945	LYS
1	C	991	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1005	LEU
1	D	667	LYS
1	D	688	GLU
1	D	693	LEU
1	D	696	MET
1	D	707	GLN
1	D	712	ILE
1	D	724	SER
1	D	729	ILE
1	D	735	ARG
1	D	747	LYS
1	D	753	ASN
1	D	779	ARG
1	D	795	GLU
1	D	805	ASP
1	D	807	ASP
1	D	809	GLU
1	D	817	TYR
1	D	833	VAL
1	D	836	ILE
1	D	886	VAL
1	D	887	THR
1	D	902	SER
1	D	903	LYS
1	D	911	SER
1	D	934	HIS
1	D	936	SER
1	D	938	ILE
1	D	939	SER
1	D	940	LYS
1	D	941	LEU
1	D	945	LYS
1	D	991	VAL
1	D	1005	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	753	ASN
1	A	759	GLN
1	A	820	ASN
1	A	846	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	853	GLN
1	A	856	ASN
1	A	862	HIS
1	A	934	HIS
1	A	937	HIS
1	A	946	HIS
1	A	961	ASN
1	A	998	ASN
1	B	753	ASN
1	B	759	GLN
1	B	820	ASN
1	B	846	GLN
1	B	853	GLN
1	B	856	ASN
1	B	862	HIS
1	B	937	HIS
1	B	946	HIS
1	B	961	ASN
1	B	998	ASN
1	C	753	ASN
1	C	759	GLN
1	C	820	ASN
1	C	846	GLN
1	C	853	GLN
1	C	856	ASN
1	C	862	HIS
1	C	875	GLN
1	C	934	HIS
1	C	937	HIS
1	C	946	HIS
1	C	961	ASN
1	C	998	ASN
1	D	753	ASN
1	D	759	GLN
1	D	820	ASN
1	D	846	GLN
1	D	853	GLN
1	D	856	ASN
1	D	862	HIS
1	D	934	HIS
1	D	937	HIS
1	D	946	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	961	ASN
1	D	998	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 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	SO4	C	2004	-	4,4,4	0.36	0	6,6,6	0.06	0
3	SO4	D	2004	-	4,4,4	0.36	0	6,6,6	0.06	0
3	SO4	D	2003	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	A	2003	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	A	2004	-	4,4,4	0.38	0	6,6,6	0.04	0
3	SO4	C	2003	-	4,4,4	0.39	0	6,6,6	0.07	0
3	SO4	D	2002	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	C	2002	-	4,4,4	0.37	0	6,6,6	0.07	0
2	UHB	C	2001	-	41,44,44	0.44	0	50,65,65	0.62	1 (2%)
3	SO4	B	2002	-	4,4,4	0.38	0	6,6,6	0.06	0
2	UHB	A	2001	-	41,44,44	0.46	0	50,65,65	0.61	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	2003	-	4,4,4	0.38	0	6,6,6	0.06	0
2	UHB	B	2001	-	41,44,44	0.46	0	50,65,65	0.63	1 (2%)
2	UHB	D	2001	-	41,44,44	0.44	0	50,65,65	0.64	1 (2%)
3	SO4	B	2004	-	4,4,4	0.37	0	6,6,6	0.07	0
3	SO4	A	2002	-	4,4,4	0.39	0	6,6,6	0.07	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
2	UHB	D	2001	-	-	1/16/55/55	0/6/6/6
2	UHB	C	2001	-	-	1/16/55/55	0/6/6/6
2	UHB	B	2001	-	-	1/16/55/55	0/6/6/6
2	UHB	A	2001	-	-	1/16/55/55	0/6/6/6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	UHB	C31-C38-N39	2.32	123.88	120.35
2	B	2001	UHB	C31-C38-N39	2.29	123.83	120.35
2	C	2001	UHB	C31-C38-N39	2.26	123.78	120.35
2	A	2001	UHB	C31-C38-N39	2.06	123.49	120.35

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	UHB	C05-C04-N11-C12
2	D	2001	UHB	C05-C04-N11-C12
2	B	2001	UHB	C05-C04-N11-C12
2	A	2001	UHB	C05-C04-N11-C12

There are no ring outliers.

4 monomers are involved in 4 short contacts:

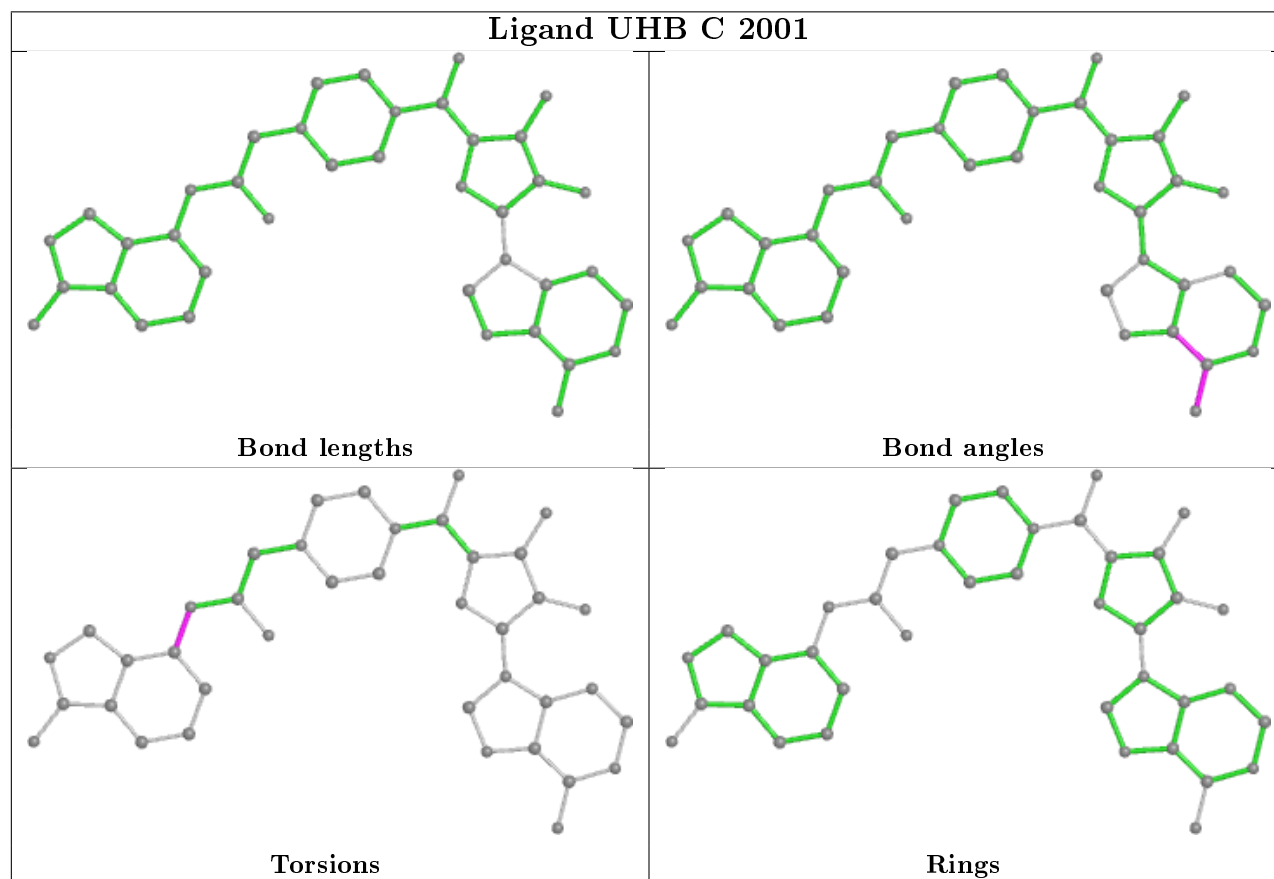
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2004	SO4	1	0

Continued on next page...

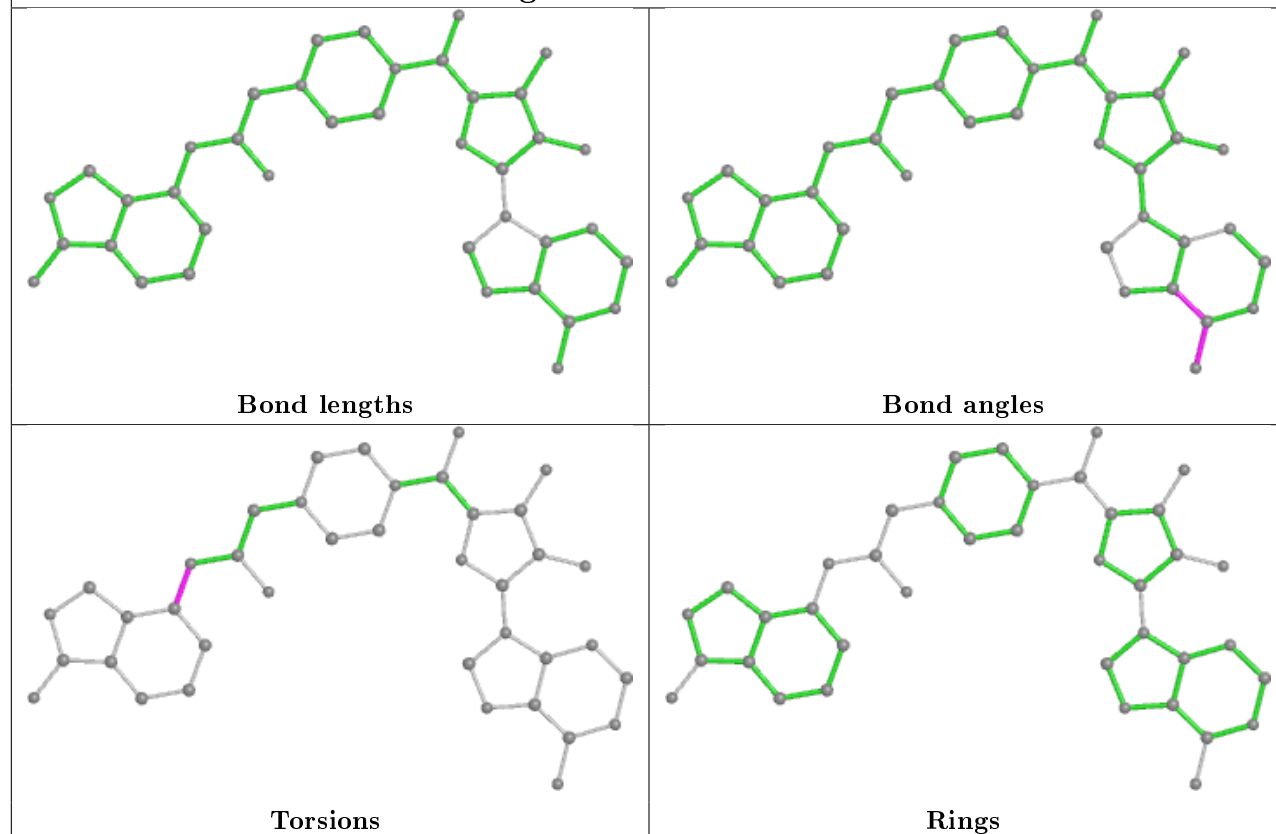
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	UHB	1	0
2	A	2001	UHB	1	0
3	B	2003	SO4	1	0

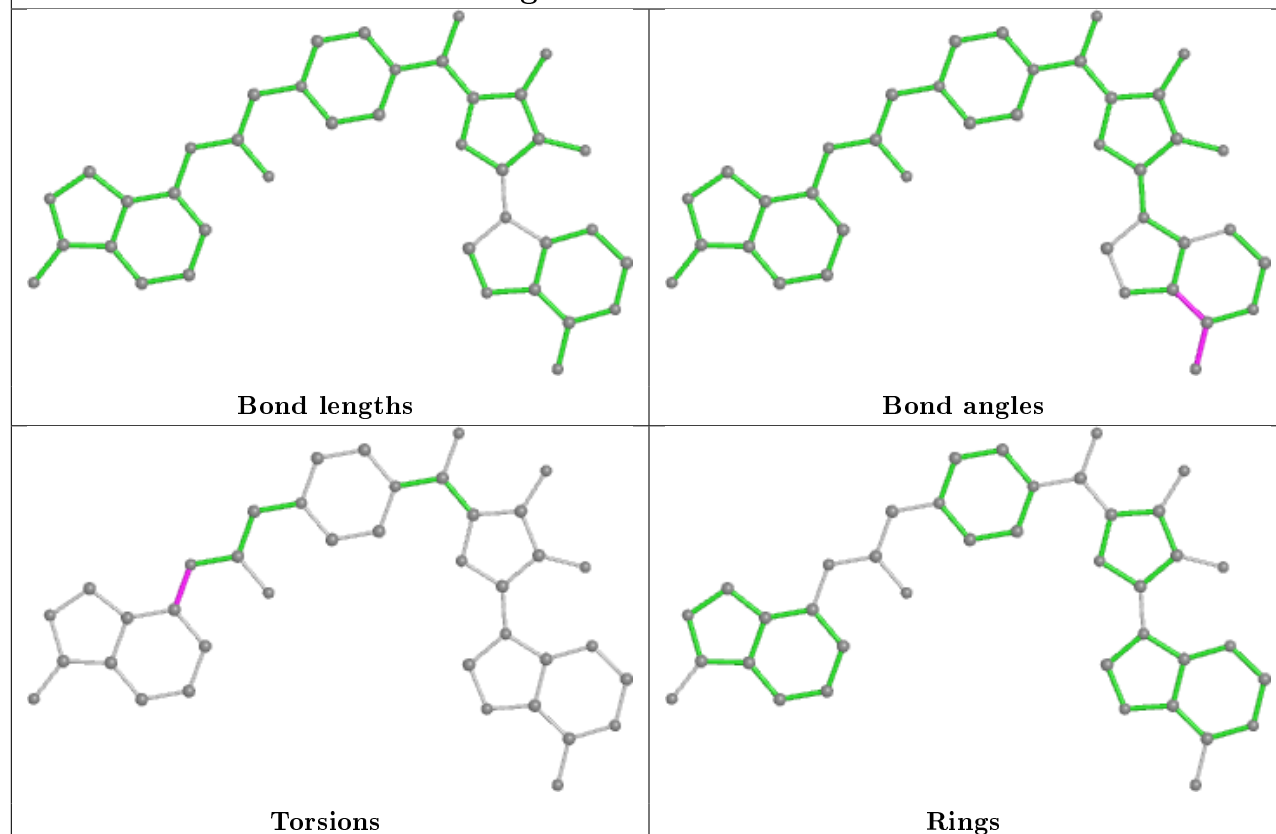
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

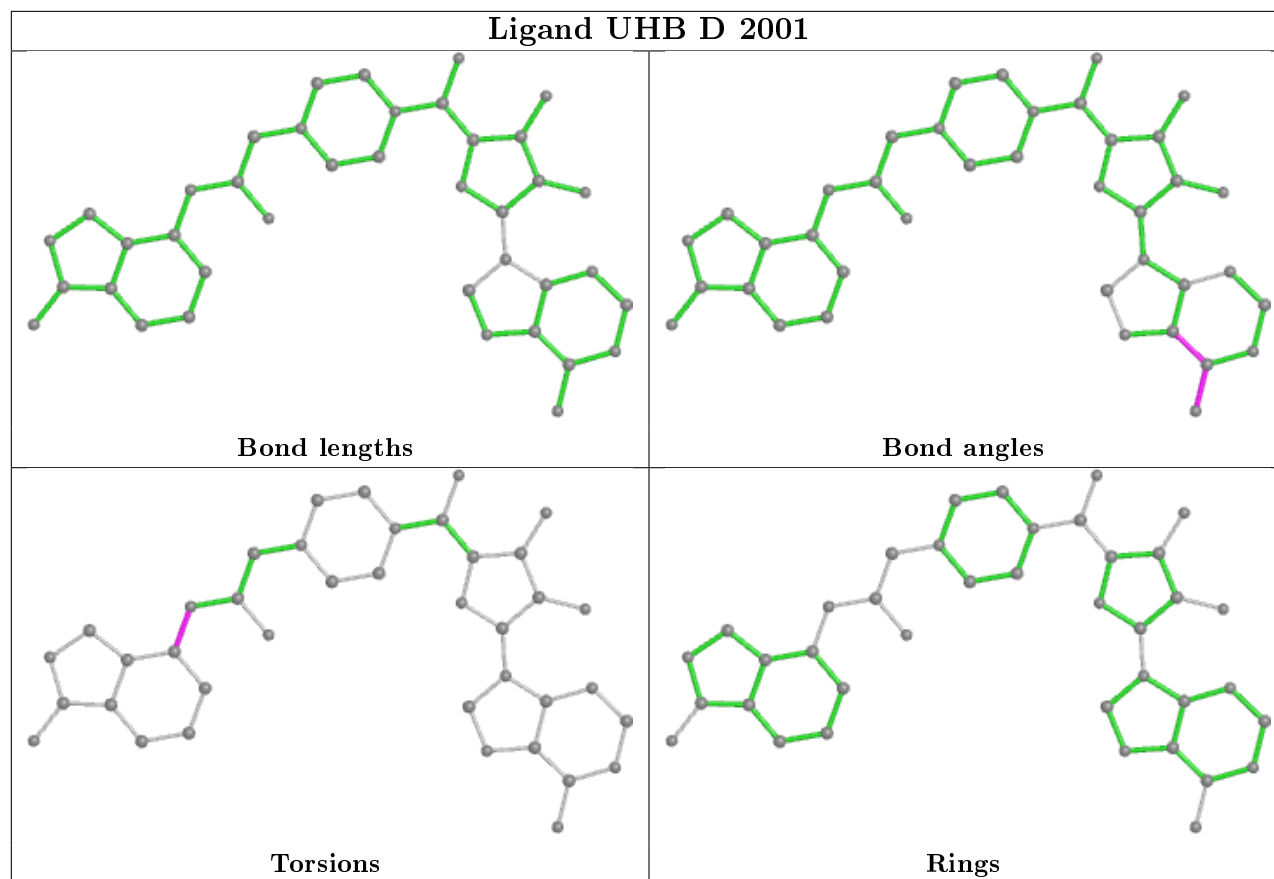


Ligand UHB A 2001



Ligand UHB B 2001





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/372 (91%)	2.03	122 (35%) 0 0	31, 74, 145, 161	0
1	B	340/372 (91%)	2.07	133 (39%) 0 0	30, 74, 148, 164	0
1	C	340/372 (91%)	1.89	118 (34%) 0 0	29, 71, 152, 165	0
1	D	340/372 (91%)	1.89	120 (35%) 0 0	28, 72, 144, 158	0
All	All	1360/1488 (91%)	1.97	493 (36%) 0 0	28, 73, 148, 165	0

All (493) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	705	GLN	13.4
1	D	1011	THR	11.1
1	A	888	GLY	11.1
1	C	752	LEU	10.9
1	B	746	MET	10.7
1	B	744	PHE	10.3
1	C	744	PHE	10.3
1	D	781	GLY	10.2
1	A	706	ILE	10.1
1	C	1011	THR	10.0
1	B	781	GLY	9.6
1	B	1011	THR	9.6
1	C	706	ILE	9.6
1	C	888	GLY	9.6
1	D	705	GLN	9.5
1	B	749	PRO	9.5
1	D	750	PRO	9.4
1	C	781	GLY	9.4
1	D	888	GLY	9.1
1	A	749	PRO	9.1
1	C	705	GLN	9.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	747	LYS	9.0
1	D	744	PHE	8.9
1	D	745	GLY	8.9
1	A	744	PHE	8.8
1	C	757	SER	8.8
1	B	888	GLY	8.8
1	A	781	GLY	8.6
1	A	752	LEU	8.5
1	A	1011	THR	8.5
1	A	705	GLN	8.4
1	B	706	ILE	8.4
1	B	750	PRO	8.3
1	B	752	LEU	8.3
1	D	752	LEU	8.2
1	A	754	ASN	8.2
1	A	750	PRO	7.9
1	C	750	PRO	7.8
1	D	706	ILE	7.4
1	C	714	SER	7.3
1	B	747	LYS	7.3
1	C	749	PRO	7.2
1	A	756	ASP	7.2
1	B	753	ASN	7.2
1	A	713	LEU	7.2
1	C	747	LYS	7.2
1	A	723	GLY	7.2
1	D	754	ASN	7.2
1	D	747	LYS	7.2
1	A	766	ASP	7.1
1	B	754	ASN	7.1
1	D	714	SER	6.9
1	A	748	LYS	6.9
1	B	688	GLU	6.8
1	C	754	ASN	6.8
1	C	713	LEU	6.7
1	C	751	LEU	6.7
1	A	689	TYR	6.7
1	D	689	TYR	6.7
1	D	713	LEU	6.7
1	A	887	THR	6.5
1	A	714	SER	6.4
1	B	745	GLY	6.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	713	LEU	6.3
1	D	753	ASN	6.2
1	C	756	ASP	6.2
1	A	743	ASP	6.1
1	B	751	LEU	5.9
1	C	753	ASN	5.9
1	B	743	ASP	5.8
1	D	699	GLY	5.7
1	A	691	ILE	5.7
1	B	693	LEU	5.7
1	C	736	PHE	5.6
1	B	756	ASP	5.6
1	B	689	TYR	5.6
1	D	887	THR	5.6
1	C	755	ALA	5.5
1	D	757	SER	5.5
1	A	693	LEU	5.5
1	B	721	SER	5.4
1	D	756	ASP	5.4
1	B	748	LYS	5.4
1	C	725	SER	5.3
1	D	736	PHE	5.3
1	A	751	LEU	5.3
1	C	748	LYS	5.2
1	A	736	PHE	5.2
1	A	746	MET	5.2
1	B	719	ALA	5.2
1	C	761	LYS	5.1
1	C	742	HIS	5.1
1	D	751	LEU	5.1
1	C	693	LEU	5.0
1	A	861	TRP	5.0
1	B	757	SER	5.0
1	C	703	LYS	5.0
1	D	704	ARG	4.9
1	D	723	GLY	4.9
1	A	818	VAL	4.8
1	A	742	HIS	4.8
1	C	689	TYR	4.8
1	D	766	ASP	4.8
1	C	723	GLY	4.8
1	A	719	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	691	ILE	4.8
1	B	1010	LYS	4.7
1	A	757	SER	4.7
1	B	714	SER	4.7
1	A	745	GLY	4.7
1	C	759	GLN	4.7
1	C	746	MET	4.7
1	B	836	ILE	4.6
1	D	755	ALA	4.6
1	B	703	LYS	4.6
1	B	726	ASP	4.6
1	D	748	LYS	4.5
1	C	726	ASP	4.5
1	C	719	ALA	4.5
1	C	688	GLU	4.5
1	B	723	GLY	4.4
1	B	769	LEU	4.4
1	B	887	THR	4.4
1	B	766	ASP	4.3
1	D	726	ASP	4.3
1	A	807	ASP	4.3
1	B	742	HIS	4.3
1	A	960	ALA	4.3
1	A	720	VAL	4.3
1	D	759	GLN	4.3
1	D	761	LYS	4.3
1	A	915	PRO	4.2
1	D	746	MET	4.2
1	B	697	PRO	4.2
1	A	753	ASN	4.2
1	D	902	SER	4.2
1	D	749	PRO	4.2
1	C	758	VAL	4.1
1	A	767	ASN	4.1
1	D	915	PRO	4.1
1	C	887	THR	4.1
1	A	721	SER	4.0
1	A	755	ALA	4.0
1	C	762	ALA	4.0
1	B	818	VAL	4.0
1	A	836	ILE	4.0
1	D	741	PRO	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	861	TRP	4.0
1	D	743	ASP	4.0
1	D	790	ILE	4.0
1	A	688	GLU	3.9
1	A	726	ASP	3.9
1	B	696	MET	3.9
1	A	704	ARG	3.8
1	D	742	HIS	3.8
1	D	721	SER	3.8
1	A	674	LYS	3.8
1	D	691	ILE	3.8
1	A	914	ASP	3.7
1	C	914	ASP	3.7
1	D	765	LEU	3.7
1	D	703	LYS	3.7
1	A	692	ASP	3.7
1	C	704	ARG	3.7
1	B	698	LEU	3.7
1	B	720	VAL	3.7
1	A	1010	LYS	3.7
1	D	963	SER	3.7
1	D	774	ALA	3.7
1	A	724	SER	3.7
1	B	699	GLY	3.7
1	C	836	ILE	3.7
1	A	981	ASP	3.6
1	C	721	SER	3.6
1	D	698	LEU	3.6
1	B	760	ALA	3.6
1	B	823	ALA	3.6
1	B	736	PHE	3.6
1	C	691	ILE	3.6
1	A	761	LYS	3.6
1	A	1009	PHE	3.6
1	D	780	GLY	3.5
1	C	963	SER	3.5
1	C	745	GLY	3.5
1	A	1005	LEU	3.5
1	D	1005	LEU	3.5
1	A	700	LYS	3.5
1	C	739	LEU	3.5
1	D	737	TYR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	700	LYS	3.5
1	B	790	ILE	3.5
1	B	761	LYS	3.5
1	B	737	TYR	3.4
1	C	735	ARG	3.4
1	C	818	VAL	3.4
1	A	823	ALA	3.4
1	A	678	ASP	3.4
1	C	738	THR	3.4
1	C	743	ASP	3.4
1	C	958	PRO	3.4
1	B	692	ASP	3.4
1	A	817	TYR	3.4
1	B	915	PRO	3.4
1	A	980	ASN	3.4
1	B	678	ASP	3.4
1	A	735	ARG	3.3
1	A	958	PRO	3.3
1	B	902	SER	3.3
1	B	729	ILE	3.3
1	B	1009	PHE	3.3
1	B	889	TYR	3.3
1	B	963	SER	3.3
1	D	823	ALA	3.3
1	C	700	LYS	3.3
1	B	739	LEU	3.3
1	A	1008	ASN	3.3
1	B	883	GLU	3.3
1	B	817	TYR	3.2
1	C	766	ASP	3.2
1	A	790	ILE	3.2
1	B	686	MET	3.2
1	A	957	ASP	3.2
1	D	729	ILE	3.2
1	A	769	LEU	3.2
1	A	696	MET	3.2
1	B	865	ARG	3.2
1	B	958	PRO	3.2
1	C	915	PRO	3.2
1	C	800	ASP	3.2
1	D	700	LYS	3.2
1	B	710	TYR	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	755	ALA	3.1
1	B	914	ASP	3.1
1	A	773	VAL	3.1
1	D	958	PRO	3.1
1	B	773	VAL	3.1
1	B	759	GLN	3.1
1	A	697	PRO	3.1
1	A	963	SER	3.1
1	D	980	ASN	3.1
1	B	695	LYS	3.1
1	B	724	SER	3.0
1	D	718	GLN	3.1
1	D	735	ARG	3.0
1	C	889	TYR	3.0
1	C	718	GLN	3.0
1	B	758	VAL	3.0
1	A	865	ARG	3.0
1	B	687	VAL	3.0
1	D	716	VAL	3.0
1	B	960	ALA	3.0
1	D	693	LEU	3.0
1	D	720	VAL	3.0
1	B	735	ARG	3.0
1	A	902	SER	3.0
1	C	667	LYS	3.0
1	B	957	ASP	3.0
1	C	699	GLY	3.0
1	B	704	ARG	3.0
1	D	948	VAL	3.0
1	A	737	TYR	3.0
1	C	1005	LEU	3.0
1	C	696	MET	3.0
1	D	836	ILE	3.0
1	A	701	LEU	2.9
1	A	718	GLN	2.9
1	C	957	ASP	2.9
1	A	729	ILE	2.9
1	C	716	VAL	2.9
1	D	957	ASP	2.9
1	D	725	SER	2.9
1	C	729	ILE	2.9
1	C	980	ASN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	730	LEU	2.9
1	C	737	TYR	2.8
1	D	817	TYR	2.8
1	C	960	ALA	2.8
1	D	861	TRP	2.8
1	C	948	VAL	2.8
1	A	681	SER	2.8
1	A	667	LYS	2.8
1	B	807	ASP	2.8
1	B	774	ALA	2.8
1	A	959	SER	2.8
1	B	804	VAL	2.8
1	D	944	GLY	2.8
1	D	962	ILE	2.8
1	D	701	LEU	2.8
1	C	817	TYR	2.8
1	D	960	ALA	2.8
1	D	975	ILE	2.7
1	A	899	ASP	2.7
1	B	959	SER	2.7
1	C	760	ALA	2.7
1	C	764	MET	2.7
1	A	703	LYS	2.7
1	A	760	ALA	2.7
1	B	764	MET	2.7
1	B	967	VAL	2.7
1	C	773	VAL	2.7
1	A	725	SER	2.7
1	B	681	SER	2.7
1	A	830	ASP	2.7
1	C	823	ALA	2.7
1	C	727	SER	2.7
1	A	716	VAL	2.7
1	B	1005	LEU	2.6
1	B	978	GLY	2.6
1	D	804	VAL	2.6
1	D	739	LEU	2.6
1	A	820	ASN	2.6
1	B	828	ALA	2.6
1	A	698	LEU	2.6
1	A	889	TYR	2.6
1	A	863	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	967	VAL	2.6
1	D	731	ASP	2.6
1	C	1008	ASN	2.6
1	C	741	PRO	2.6
1	A	962	ILE	2.6
1	D	936	SER	2.6
1	D	959	SER	2.6
1	A	916	ILE	2.6
1	C	902	SER	2.6
1	B	767	ASN	2.6
1	D	762	ALA	2.6
1	A	695	LYS	2.6
1	A	759	GLN	2.6
1	D	740	ILE	2.6
1	B	765	LEU	2.6
1	B	718	GLN	2.6
1	B	722	GLN	2.6
1	B	936	SER	2.6
1	C	730	LEU	2.5
1	D	688	GLU	2.5
1	A	1004	LYS	2.5
1	D	767	ASN	2.5
1	D	801	ILE	2.5
1	A	665	LEU	2.5
1	C	804	VAL	2.5
1	B	727	SER	2.5
1	B	976	SER	2.5
1	D	724	SER	2.5
1	B	975	ILE	2.5
1	B	980	ASN	2.5
1	C	962	ILE	2.5
1	D	899	ASP	2.5
1	A	832	GLU	2.5
1	A	672	LEU	2.5
1	B	685	ALA	2.5
1	C	967	VAL	2.5
1	A	971	LEU	2.5
1	D	818	VAL	2.5
1	D	937	HIS	2.5
1	D	728	GLN	2.5
1	C	979	VAL	2.5
1	C	724	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	820	ASN	2.4
1	B	837	PHE	2.4
1	C	670	GLN	2.4
1	C	936	SER	2.4
1	D	947	SER	2.4
1	C	722	GLN	2.4
1	D	677	PHE	2.4
1	D	758	VAL	2.4
1	B	832	GLU	2.4
1	C	861	TRP	2.4
1	C	947	SER	2.4
1	B	780	GLY	2.4
1	B	913	GLY	2.4
1	D	865	ARG	2.4
1	D	719	ALA	2.4
1	A	765	LEU	2.4
1	A	853	GLN	2.4
1	B	674	LYS	2.4
1	D	932	LEU	2.4
1	A	917	GLY	2.4
1	C	937	HIS	2.4
1	B	679	VAL	2.4
1	C	710	TYR	2.4
1	C	821	THR	2.4
1	B	762	ALA	2.4
1	C	959	SER	2.4
1	C	938	ILE	2.4
1	B	815	ARG	2.4
1	C	1010	LYS	2.4
1	D	795	GLU	2.4
1	B	937	HIS	2.3
1	D	979	VAL	2.3
1	C	807	ASP	2.3
1	C	711	SER	2.3
1	C	827	ASN	2.3
1	C	840	GLU	2.3
1	A	979	VAL	2.3
1	B	694	GLN	2.3
1	C	815	ARG	2.3
1	A	936	SER	2.3
1	C	790	ILE	2.3
1	A	815	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	979	VAL	2.3
1	A	722	GLN	2.3
1	D	773	VAL	2.3
1	A	730	LEU	2.3
1	A	828	ALA	2.3
1	D	967	VAL	2.3
1	A	913	GLY	2.3
1	C	853	GLN	2.3
1	C	763	GLU	2.3
1	D	914	ASP	2.3
1	B	962	ILE	2.3
1	D	696	MET	2.3
1	A	837	PHE	2.3
1	A	738	THR	2.2
1	B	821	THR	2.2
1	C	697	PRO	2.2
1	D	710	TYR	2.2
1	B	853	GLN	2.2
1	B	1008	ASN	2.2
1	C	865	ARG	2.2
1	B	860	LEU	2.2
1	B	863	GLY	2.2
1	D	889	TYR	2.2
1	D	734	ASN	2.2
1	B	690	GLU	2.2
1	C	886	VAL	2.2
1	D	820	ASN	2.2
1	C	860	LEU	2.2
1	C	917	GLY	2.2
1	C	981	ASP	2.2
1	A	860	LEU	2.2
1	D	711	SER	2.2
1	D	764	MET	2.2
1	A	819	LYS	2.2
1	B	824	THR	2.2
1	D	769	LEU	2.2
1	D	891	PHE	2.2
1	C	832	GLU	2.2
1	C	830	ASP	2.2
1	A	686	MET	2.2
1	A	885	PRO	2.2
1	C	690	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	695	LYS	2.2
1	B	899	ASP	2.2
1	D	791	ASP	2.2
1	D	800	ASP	2.2
1	A	814	ILE	2.2
1	B	930	TYR	2.2
1	D	978	GLY	2.2
1	A	937	HIS	2.2
1	B	779	ARG	2.2
1	B	806	ARG	2.2
1	B	973	THR	2.1
1	D	974	GLY	2.1
1	C	698	LEU	2.1
1	B	667	LYS	2.1
1	A	668	PRO	2.1
1	B	947	SER	2.1
1	C	899	ASP	2.1
1	D	671	ASP	2.1
1	B	948	VAL	2.1
1	C	780	GLY	2.1
1	A	763	GLU	2.1
1	A	930	TYR	2.1
1	B	701	LEU	2.1
1	A	901	VAL	2.1
1	C	822	HIS	2.1
1	B	954	THR	2.1
1	C	932	LEU	2.1
1	D	971	LEU	2.1
1	B	800	ASP	2.1
1	C	845	CYS	2.1
1	A	975	ILE	2.1
1	D	863	GLY	2.1
1	B	932	LEU	2.1
1	D	853	GLN	2.1
1	D	981	ASP	2.1
1	B	716	VAL	2.1
1	B	665	LEU	2.0
1	D	770	ASP	2.0
1	D	1010	LYS	2.0
1	A	804	VAL	2.0
1	C	891	PHE	2.0
1	D	972	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	910	THR	2.0
1	D	827	ASN	2.0
1	B	668	PRO	2.0
1	C	971	LEU	2.0
1	C	678	ASP	2.0
1	A	898	ALA	2.0
1	B	939	SER	2.0
1	D	760	ALA	2.0
1	C	686	MET	2.0
1	D	722	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
2	UHB	A	2001	39/39	0.79	0.37	49,77,83,83	0
2	UHB	B	2001	39/39	0.81	0.33	51,81,88,88	0
2	UHB	D	2001	39/39	0.81	0.33	43,76,86,86	0
3	SO4	D	2002	5/5	0.82	0.28	75,76,80,80	0
3	SO4	C	2002	5/5	0.82	0.30	77,77,79,81	0
2	UHB	C	2001	39/39	0.82	0.31	38,74,81,82	0
3	SO4	A	2002	5/5	0.86	0.27	77,78,80,83	0
3	SO4	B	2002	5/5	0.87	0.29	74,74,76,79	0
3	SO4	A	2003	5/5	0.87	0.23	67,69,72,74	0
3	SO4	C	2004	5/5	0.87	0.24	57,58,63,63	0
3	SO4	B	2003	5/5	0.88	0.26	73,75,78,78	0
3	SO4	C	2003	5/5	0.89	0.23	67,67,69,71	0
3	SO4	B	2004	5/5	0.92	0.22	56,60,62,65	0

Continued on next page...

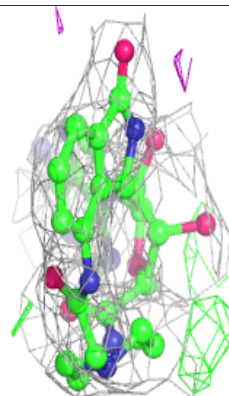
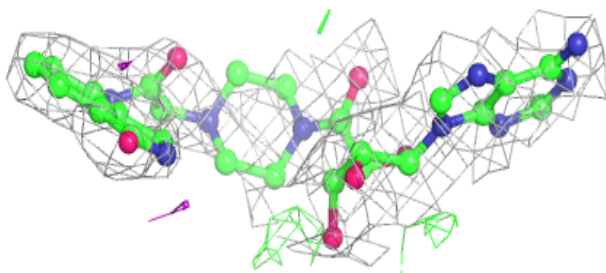
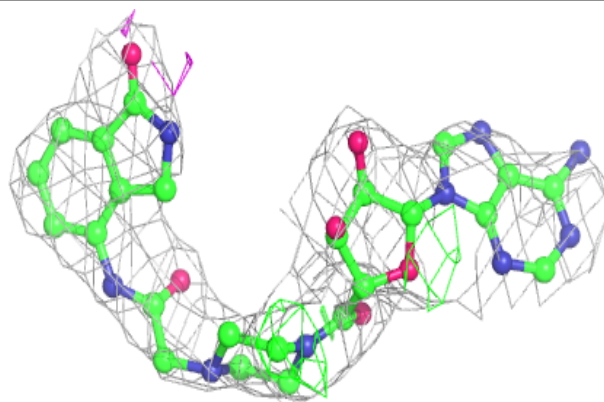
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	2004	5/5	0.93	0.21	57,62,62,63	0
3	SO4	D	2003	5/5	0.93	0.18	65,65,67,68	0
3	SO4	D	2004	5/5	0.93	0.20	55,58,62,63	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.

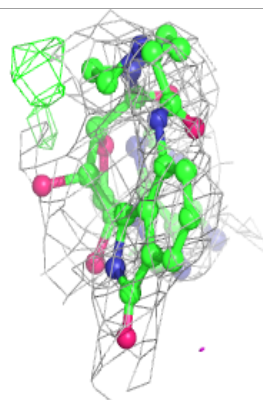
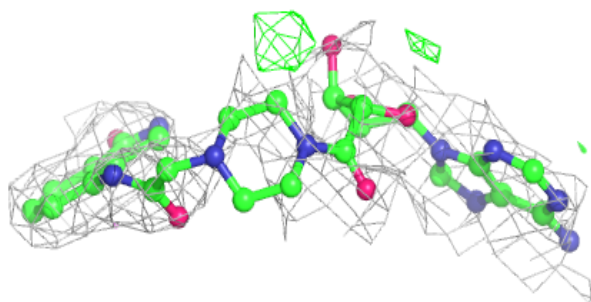
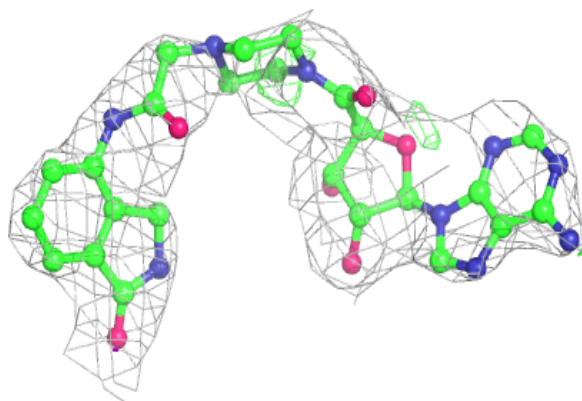
Electron density around UHB A 2001:

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

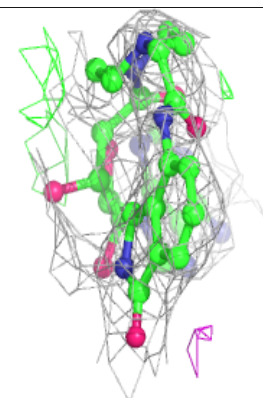
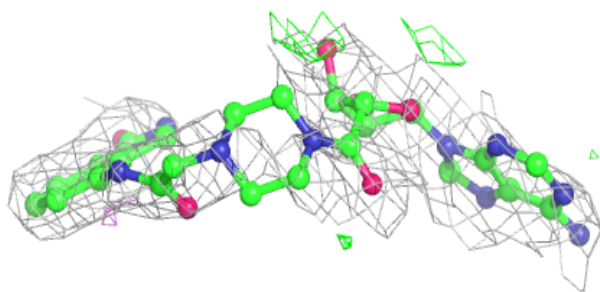
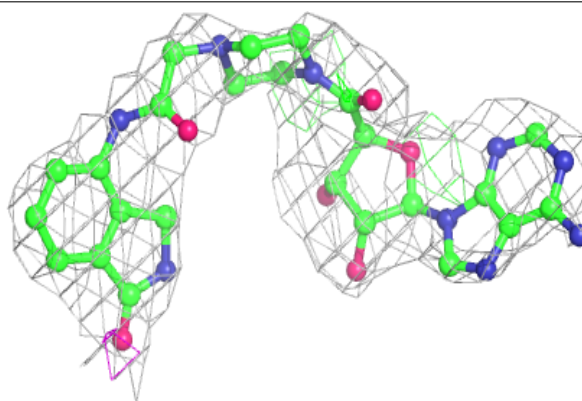


Electron density around UHB B 2001:

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

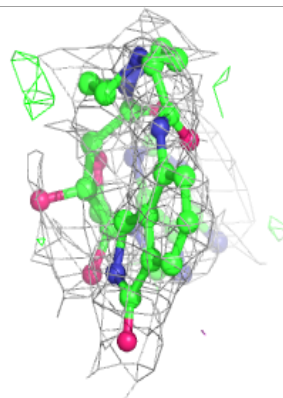
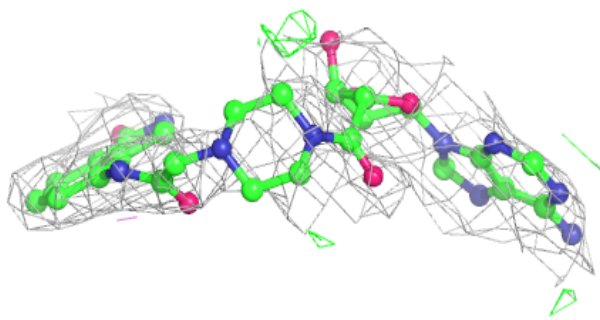
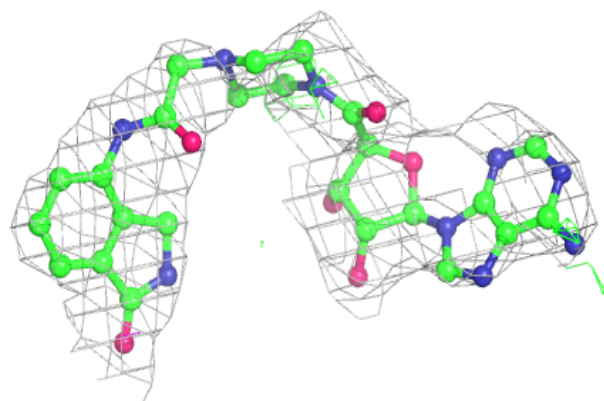
**Electron density around UHB D 2001:**

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



Electron density around UHB C 2001:

$2mF_o-DF_c$ (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.