



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:05 PM UTC

PDB ID : 6VKQ / pdb_00006vkq
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

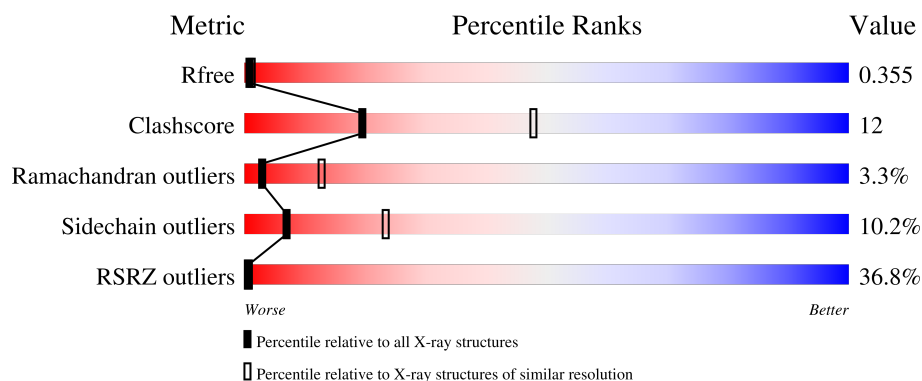
1 Overall quality at a glance

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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 $\leq 5\%$. 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	33% 61% 27% 9%
1	B	372	36% 62% 26% 9%
1	C	372	31% 61% 26% 9%
1	D	372	34% 63% 24% 9%

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

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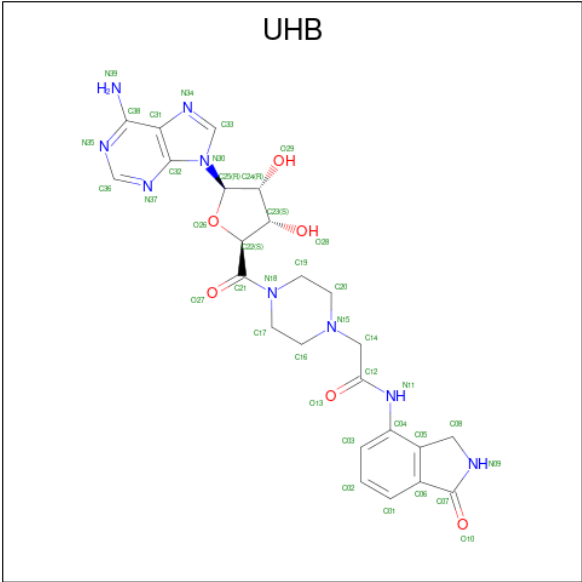
Chain	Residue	Modelled	Actual	Comment	Reference
A	762	ALA	VAL	variant	UNP P09874
B	640	MET	-	initiating methionine	UNP P09874
B	641	GLY	-	expression tag	UNP P09874
B	642	SER	-	expression tag	UNP P09874
B	643	SER	-	expression tag	UNP P09874
B	644	HIS	-	expression tag	UNP P09874
B	645	HIS	-	expression 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

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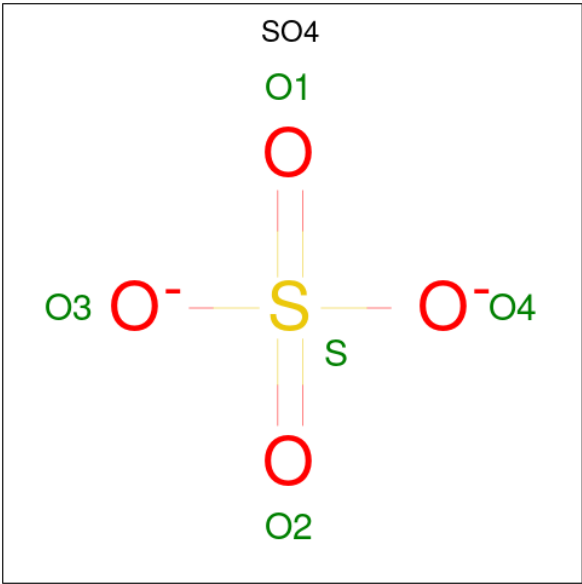
Chain	Residue	Modelled	Actual	Comment	Reference
C	659	HIS	-	expression tag	UNP P09874
C	660	MET	-	expression tag	UNP P09874
C	762	ALA	VAL	variant	UNP P09874
D	640	MET	-	initiating methionine	UNP P09874
D	641	GLY	-	expression tag	UNP P09874
D	642	SER	-	expression tag	UNP P09874
D	643	SER	-	expression 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-dihydroisoindol-4-yl)ethanamide (CCD ID: UHB) (formula: C₂₄H₂₇N₉O₆) (labeled as "Ligand of Interest" by depositor).



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 (CCD ID: SO4) (formula: O₄S).

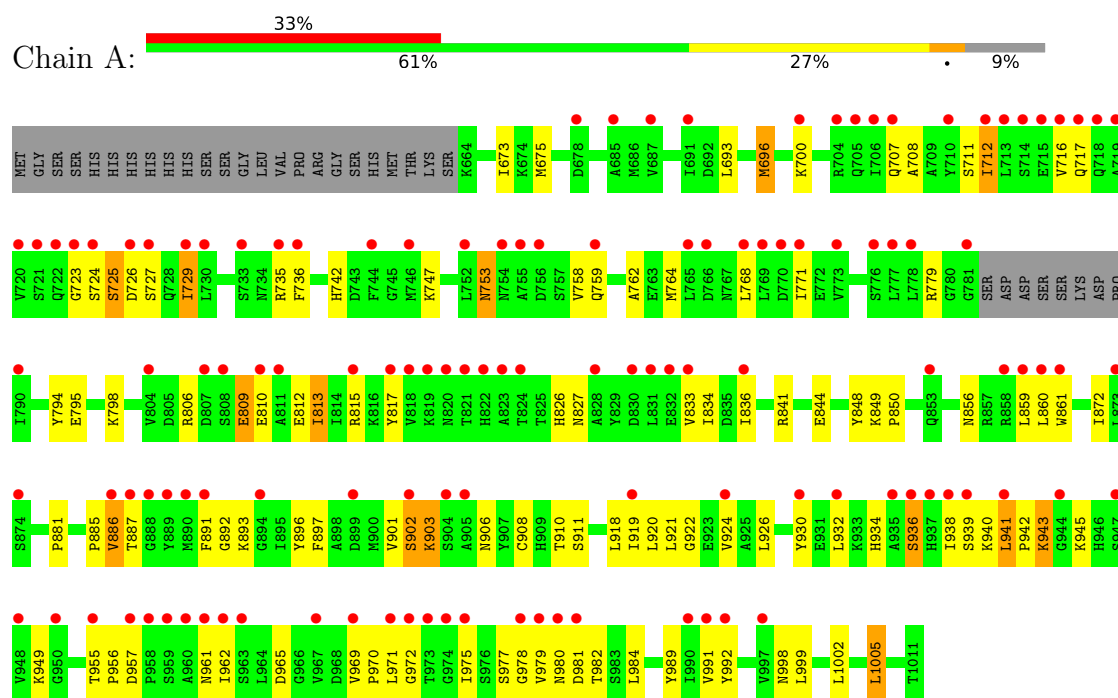


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

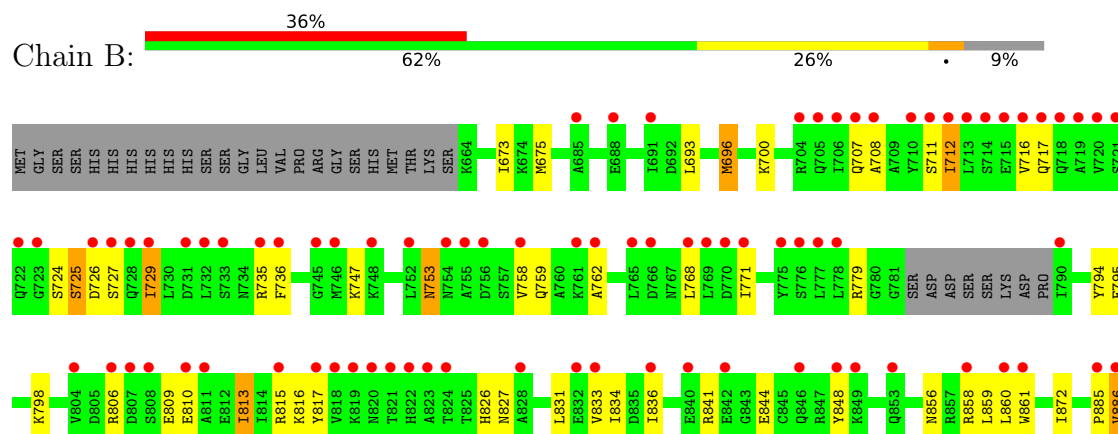
3 Residue-property plots

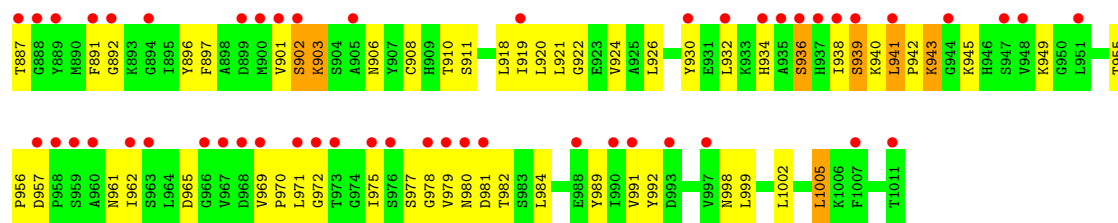
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

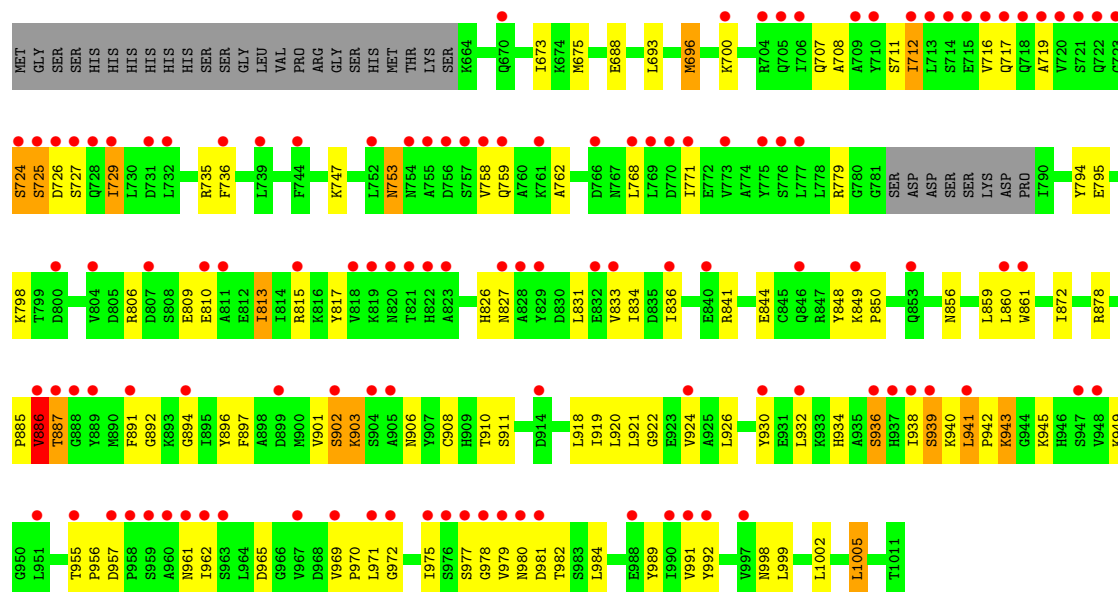


• Molecule 1: Poly [ADP-ribose] polymerase 1

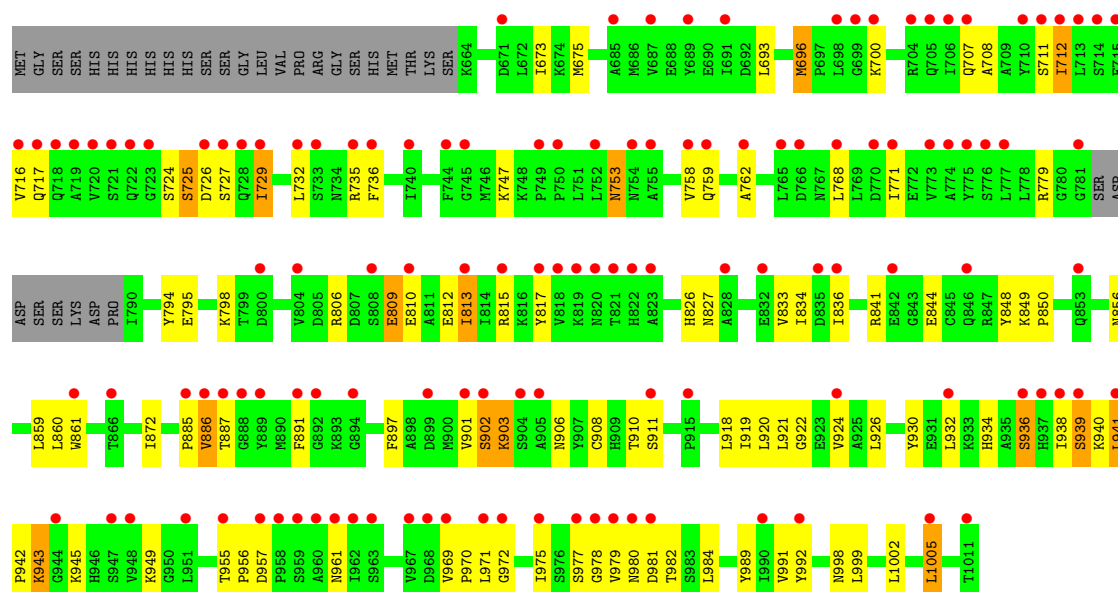




• Molecule 1: Poly [ADP-ribose] polymerase 1



• 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 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.90) 99.0 (20.00-2.90)	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	1916 reflections (5.06%)	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)	0.32 , 68.4	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: SO4, UHB

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	1.05	0/2728	1.45	0/3681
1	B	1.06	0/2722	1.45	0/3674
1	C	1.06	0/2722	1.45	1/3674 (0.0%)
1	D	1.06	0/2722	1.46	0/3674
All	All	1.06	0/10894	1.45	1/14703 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	894	GLY	CA-C-O	-5.11	116.82	121.47

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	67	0
1	B	2672	0	2714	65	0
1	C	2672	0	2714	67	0
1	D	2672	0	2714	63	0
2	A	39	0	27	1	0
2	B	39	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	39	0	27	1	0
2	D	39	0	27	0	0
3	A	15	0	0	1	0
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	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (254) 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:977:SER:C	1:D:979:VAL:H	2.07	0.62
1:B:977:SER:C	1:B:979:VAL:H	2.07	0.62
1:D:860:LEU:HD12	1:D:924:VAL:CG2	2.30	0.62
1:A:977:SER:C	1:A:979:VAL:H	2.07	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:977:SER:C	1:C:979:VAL:H	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:D:980:ASN:C	1:D:982:THR:H	2.15	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:B:980:ASN:C	1:B:982:THR:H	2.15	0.53
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:A:980:ASN:C	1:A:982:THR:H	2.15	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:C:980:ASN:C	1:C:982:THR:H	2.15	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:753:ASN:H	1:D:753:ASN:HD22	1.59	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:725:SER:C	1:B:729:ILE:HG13	2.37	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:D:725:SER:C	1:D:729:ILE:HG13	2.37	0.50
1:A:725:SER:C	1:A:729:ILE:HG13	2.37	0.49
1:A:860:LEU:HD12	1:A:924:VAL:HG21	1.94	0.49
1:C:753:ASN:HD22	1:C:753:ASN:H	1.59	0.49
1:D:980:ASN:O	1:D:982:THR:N	2.35	0.49
1:C:725:SER:C	1:C:729:ILE:HG13	2.37	0.49
1:A:768:LEU:HA	1:A:771:ILE:HB	1.95	0.49
1:A:753:ASN:H	1:A:753:ASN:HD22	1.59	0.49
1:B:768:LEU:HA	1:B:771:ILE:HB	1.95	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: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:A:708:ALA:O	1:A:711:SER:OG	2.27	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: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:817:TYR:CE1	1:D:970:PRO:O	2.67	0.47
1:D:919:ILE:HG21	1:D:1005:LEU:HD21	1.97	0.47
1:A:848:TYR:CG	1:A:998:ASN:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:892:GLY:O	1:B:896:TYR:OH	2.18	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
1:C:813:ILE:HD13	1:C:813:ILE:N	2.31	0.46
1:A:675:MET:HE1	1:A:918:LEU:HD21	1.98	0.45
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:HD13	1:A:813:ILE:N	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:965:ASP:HA	1:C:942:PRO:HA	1.97	0.45
1:C:919:ILE:HG21	1:C:1005:LEU:HD21	1.98	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:712:ILE:HD12	1:D:735:ARG:HD2	1.98	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: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:696:MET:HE2	1:B:700:LYS:HB3	2.00	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:708:ALA:O	1:B:711:SER:OG	2.26	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:MET:HE1	1:B:918:LEU:HD21	2.00	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:C:708:ALA:O	1:C:711:SER:OG	2.27	0.44
1:D:708:ALA:O	1:D:711:SER:OG	2.27	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
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:D:980:ASN:C	1:D:982:THR:N	2.76	0.44
1:B:980:ASN:C	1:B:982:THR:N	2.76	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:C:980:ASN:C	1:C:982:THR:N	2.76	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:956:PRO:O	1:A:957:ASP:C	2.61	0.43
1:B:956:PRO:O	1:B:957:ASP:C	2.61	0.43
1:D:977:SER:C	1:D:979:VAL:N	2.72	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:C:956:PRO:O	1:C:957:ASP:C	2.61	0.43
1:D:696:MET:HE2	1:D:700:LYS:HB3	2.00	0.43
1:D:903:LYS:HA	1:D:906:ASN:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:ASP:HA	1:B:942:PRO:HA	2.00	0.43
1:B:858:ARG:NH2	3:B:2003:SO4:O4	2.52	0.43
1:C:675:MET:HE1	1:C:918:LEU:HD21	1.99	0.43
1:A:903:LYS:HA	1:A:906:ASN:HD22	1.84	0.43
1:A:942:PRO:O	1:A:943:LYS:C	2.62	0.43
1:A:980:ASN:C	1:A:982:THR:N	2.76	0.43
1:C:919:ILE:CG2	1:C:1005:LEU:HD21	2.49	0.43
1:D:956:PRO:O	1:D:957:ASP:C	2.61	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:C:696:MET:HE2	1:C:700:LYS:HB3	2.00	0.42
1:D:673:ILE:HD13	1:D:794:TYR:HB2	2.02	0.42
1:A:696:MET:HE2	1:A:700:LYS:HB3	2.01	0.42
1:A:956:PRO:HB3	1:A:972:GLY:C	2.45	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:B:942:PRO:O	1:B:943:LYS:C	2.62	0.42
1:C:1002:LEU:HD23	1:C:1002:LEU:C	2.45	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:D:956:PRO:HB3	1:D:972:GLY:C	2.45	0.42
1:C:942:PRO:O	1:C:943:LYS:C	2.62	0.41
1:C:965:ASP:HA	1:D:942:PRO:HA	2.02	0.41
1:D:942:PRO:O	1:D:943:LYS:C	2.63	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
1:A:961:ASN:CG	1:A:970:PRO:HA	2.46	0.41
1:C:956:PRO:HB3	1:C:972:GLY:C	2.45	0.41
1:A:717:GLN:OE1	1:A:758:VAL:HG11	2.20	0.41
1:B:956:PRO:HB3	1:B:972:GLY:C	2.45	0.41
1:D:725:SER:O	1:D:727:SER:N	2.53	0.41
1:B:831:LEU:HD12	1:B:831:LEU:HA	1.92	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:C:961:ASN:CG	1:C:970:PRO:HA	2.46	0.41
1:D:675:MET:HE1	1:D:918:LEU:HD21	2.01	0.41
1:A:742:HIS:CE1	1:A:764:MET:HE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:SER:C	1:A:979:VAL:N	2.72	0.41
1:B:961:ASN:CG	1:B:970:PRO:HA	2.46	0.41
1:B:1002:LEU:HD23	1:B:1002:LEU:C	2.45	0.41
1:C:717:GLN:OE1	1:C:758:VAL:HG11	2.20	0.41
1:D:930:TYR:CE1	1:D:932:LEU:HD21	2.56	0.41
1:D:961:ASN:CG	1:D:970:PRO:HA	2.45	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:B:815:ARG:O	1:B:816:LYS:C	2.64	0.40
1:A:962:ILE:CG2	1:B:939:SER:HB2	2.43	0.40
1:C:831:LEU:HD12	1:C:831:LEU:HA	1.93	0.40
1:D:1002:LEU:C	1:D:1002:LEU:HD23	2.46	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:A:849:LYS:NZ	3:A:2004:SO4:O4	2.49	0.40
1:A:1002:LEU:HD23	1:A:1002:LEU:C	2.46	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%)	2	11
1	B	336/372 (90%)	287 (85%)	38 (11%)	11 (3%)	3	13
1	C	336/372 (90%)	288 (86%)	37 (11%)	11 (3%)	3	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	336/372 (90%)	287 (85%)	38 (11%)	11 (3%)	3	13
All	All	1344/1488 (90%)	1150 (86%)	149 (11%)	45 (3%)	3	13

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
1	A	798	LYS
1	B	725	SER

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Mol	Chain	Res	Type
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%)	267 (90%)	30 (10%)	7	24
1	B	296/326 (91%)	266 (90%)	30 (10%)	7	24
1	C	296/326 (91%)	265 (90%)	31 (10%)	6	22
1	D	296/326 (91%)	266 (90%)	30 (10%)	7	24
All	All	1185/1304 (91%)	1064 (90%)	121 (10%)	7	23

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	747	LYS
1	A	753	ASN
1	A	779	ARG
1	A	795	GLU
1	A	809	GLU
1	A	813	ILE

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Mol	Chain	Res	Type
1	A	827	ASN
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	941	LEU
1	A	945	LYS
1	A	949	LYS
1	A	984	LEU
1	A	991	VAL
1	A	1005	LEU
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	747	LYS
1	B	753	ASN
1	B	779	ARG
1	B	795	GLU
1	B	809	GLU
1	B	813	ILE
1	B	827	ASN
1	B	833	VAL
1	B	836	ILE
1	B	886	VAL
1	B	887	THR
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

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Mol	Chain	Res	Type
1	B	941	LEU
1	B	945	LYS
1	B	949	LYS
1	B	984	LEU
1	B	991	VAL
1	B	1005	LEU
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	747	LYS
1	C	753	ASN
1	C	779	ARG
1	C	795	GLU
1	C	809	GLU
1	C	813	ILE
1	C	827	ASN
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	941	LEU
1	C	945	LYS
1	C	949	LYS
1	C	984	LEU
1	C	991	VAL
1	C	1005	LEU
1	D	693	LEU
1	D	696	MET
1	D	707	GLN
1	D	712	ILE
1	D	724	SER

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Mol	Chain	Res	Type
1	D	729	ILE
1	D	747	LYS
1	D	753	ASN
1	D	779	ARG
1	D	795	GLU
1	D	809	GLU
1	D	813	ILE
1	D	827	ASN
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	941	LEU
1	D	945	LYS
1	D	949	LYS
1	D	984	LEU
1	D	991	VAL
1	D	1005	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	705	GLN
1	A	728	GLN
1	A	753	ASN
1	A	820	ASN
1	A	853	GLN
1	A	862	HIS
1	A	868	ASN
1	A	909	HIS
1	A	937	HIS
1	A	946	HIS
1	A	961	ASN
1	A	996	GLN
1	A	998	ASN

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Mol	Chain	Res	Type
1	B	705	GLN
1	B	728	GLN
1	B	753	ASN
1	B	820	ASN
1	B	846	GLN
1	B	853	GLN
1	B	862	HIS
1	B	909	HIS
1	B	937	HIS
1	B	946	HIS
1	B	961	ASN
1	B	996	GLN
1	B	998	ASN
1	C	705	GLN
1	C	728	GLN
1	C	753	ASN
1	C	820	ASN
1	C	846	GLN
1	C	853	GLN
1	C	862	HIS
1	C	868	ASN
1	C	875	GLN
1	C	909	HIS
1	C	937	HIS
1	C	946	HIS
1	C	961	ASN
1	C	996	GLN
1	C	998	ASN
1	C	1008	ASN
1	D	705	GLN
1	D	728	GLN
1	D	753	ASN
1	D	820	ASN
1	D	846	GLN
1	D	853	GLN
1	D	862	HIS
1	D	868	ASN
1	D	875	GLN
1	D	909	HIS
1	D	937	HIS
1	D	946	HIS
1	D	961	ASN

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Mol	Chain	Res	Type
1	D	996	GLN
1	D	998	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	2003	-	4,4,4	0.35	0	6,6,6	0.05	0
3	SO4	A	2003	-	4,4,4	0.32	0	6,6,6	0.11	0
3	SO4	D	2002	-	4,4,4	0.33	0	6,6,6	0.11	0
3	SO4	D	2003	-	4,4,4	0.34	0	6,6,6	0.09	0
2	UHB	D	2001	-	44,44,44	0.17	0	62,65,65	0.55	1 (1%)
2	UHB	C	2001	-	44,44,44	0.17	0	62,65,65	0.53	1 (1%)
2	UHB	B	2001	-	44,44,44	0.18	0	62,65,65	0.54	1 (1%)
3	SO4	D	2004	-	4,4,4	0.32	0	6,6,6	0.09	0
3	SO4	B	2002	-	4,4,4	0.33	0	6,6,6	0.08	0
3	SO4	A	2004	-	4,4,4	0.35	0	6,6,6	0.07	0
3	SO4	C	2002	-	4,4,4	0.32	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UHB	A	2001	-	44,44,44	0.18	0	62,65,65	0.54	1 (1%)
3	SO4	B	2003	-	4,4,4	0.34	0	6,6,6	0.05	0
3	SO4	A	2002	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	B	2004	-	4,4,4	0.34	0	6,6,6	0.09	0
3	SO4	C	2004	-	4,4,4	0.33	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	-	-	4/20/55/55	0/6/6/6
2	UHB	C	2001	-	-	3/20/55/55	0/6/6/6
2	UHB	B	2001	-	-	4/20/55/55	0/6/6/6
2	UHB	A	2001	-	-	5/20/55/55	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	C06-C05-C04	-2.44	119.83	120.97
2	A	2001	UHB	C06-C05-C04	-2.30	119.89	120.97
2	C	2001	UHB	C06-C05-C04	-2.28	119.90	120.97
2	B	2001	UHB	C06-C05-C04	-2.28	119.91	120.97

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	UHB	O26-C25-N30-C33
2	C	2001	UHB	O26-C25-N30-C32
2	D	2001	UHB	O26-C25-N30-C32
2	D	2001	UHB	O26-C25-N30-C33
2	B	2001	UHB	O26-C25-N30-C33
2	B	2001	UHB	O26-C25-N30-C32
2	A	2001	UHB	O26-C25-N30-C33
2	A	2001	UHB	C24-C25-N30-C33
2	C	2001	UHB	C05-C04-N11-C12
2	A	2001	UHB	C24-C25-N30-C32

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Mol	Chain	Res	Type	Atoms
2	A	2001	UHB	O26-C25-N30-C32
2	D	2001	UHB	C05-C04-N11-C12
2	D	2001	UHB	C24-C25-N30-C33
2	A	2001	UHB	C05-C04-N11-C12
2	B	2001	UHB	C05-C04-N11-C12
2	B	2001	UHB	C24-C25-N30-C33

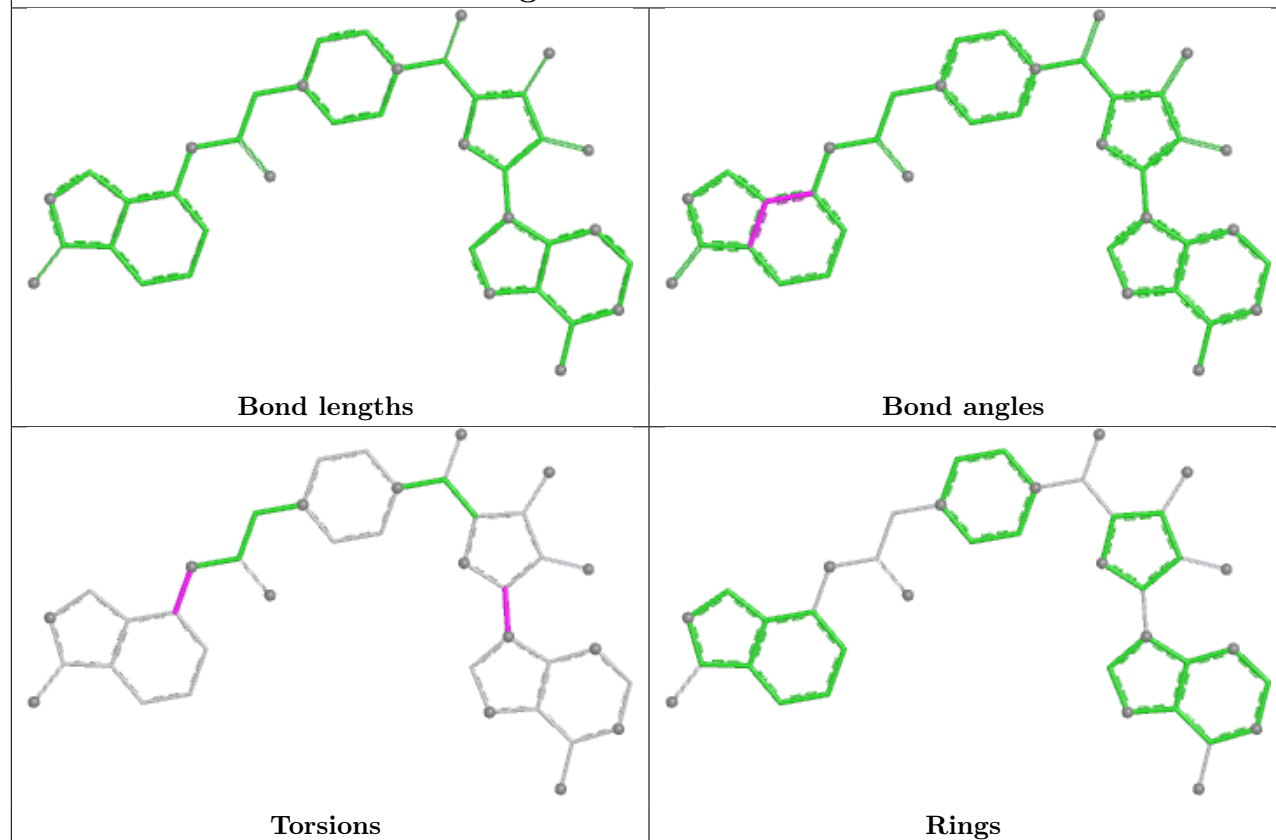
There are no ring outliers.

4 monomers are involved in 4 short contacts:

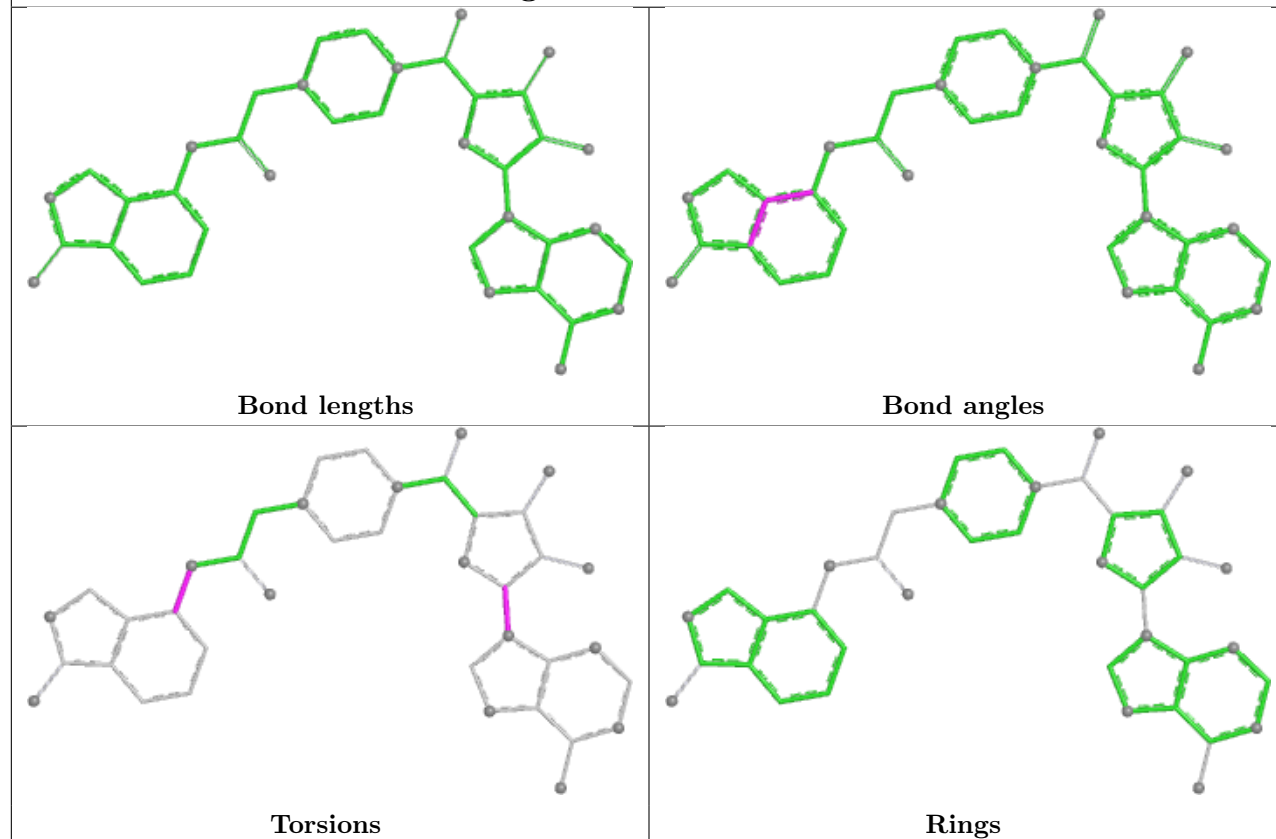
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2001	UHB	1	0
3	A	2004	SO4	1	0
2	A	2001	UHB	1	0
3	B	2003	SO4	1	0

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.

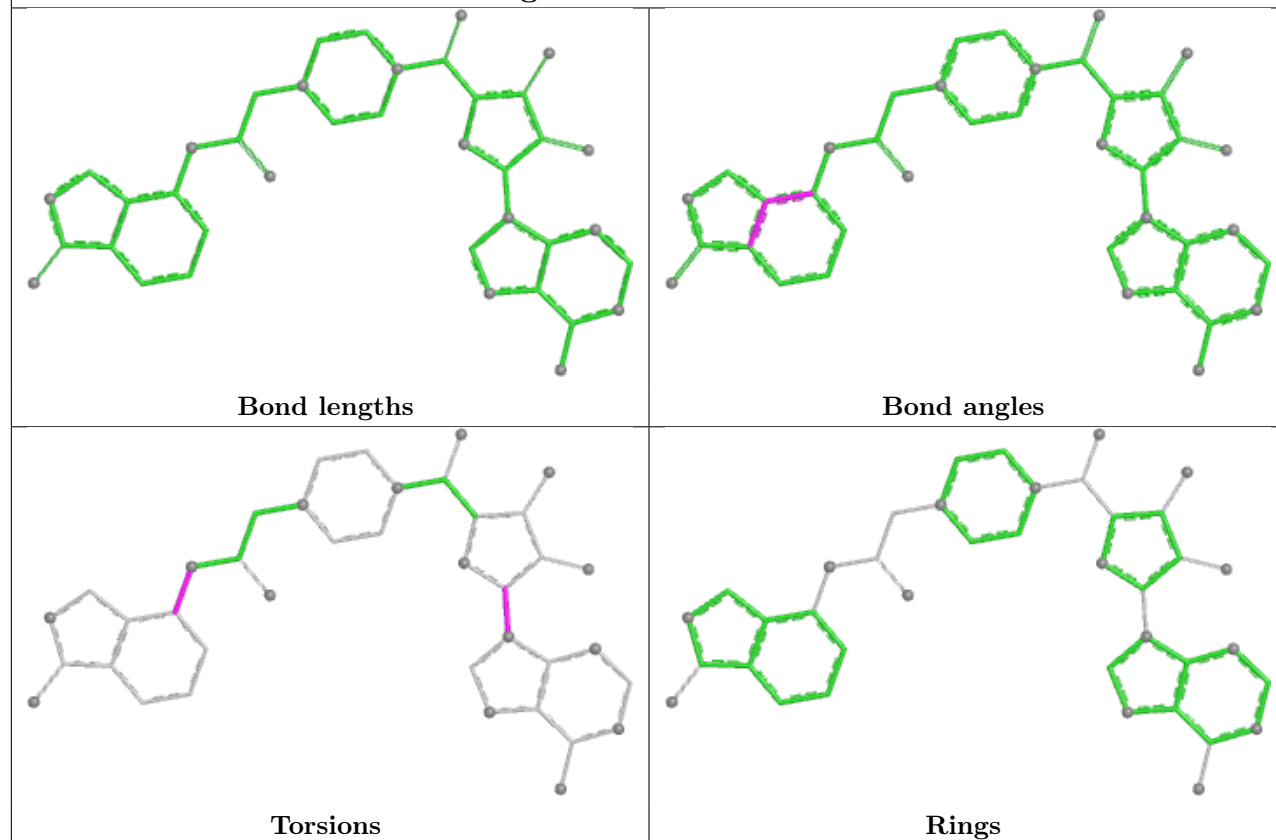
Ligand UHB D 2001



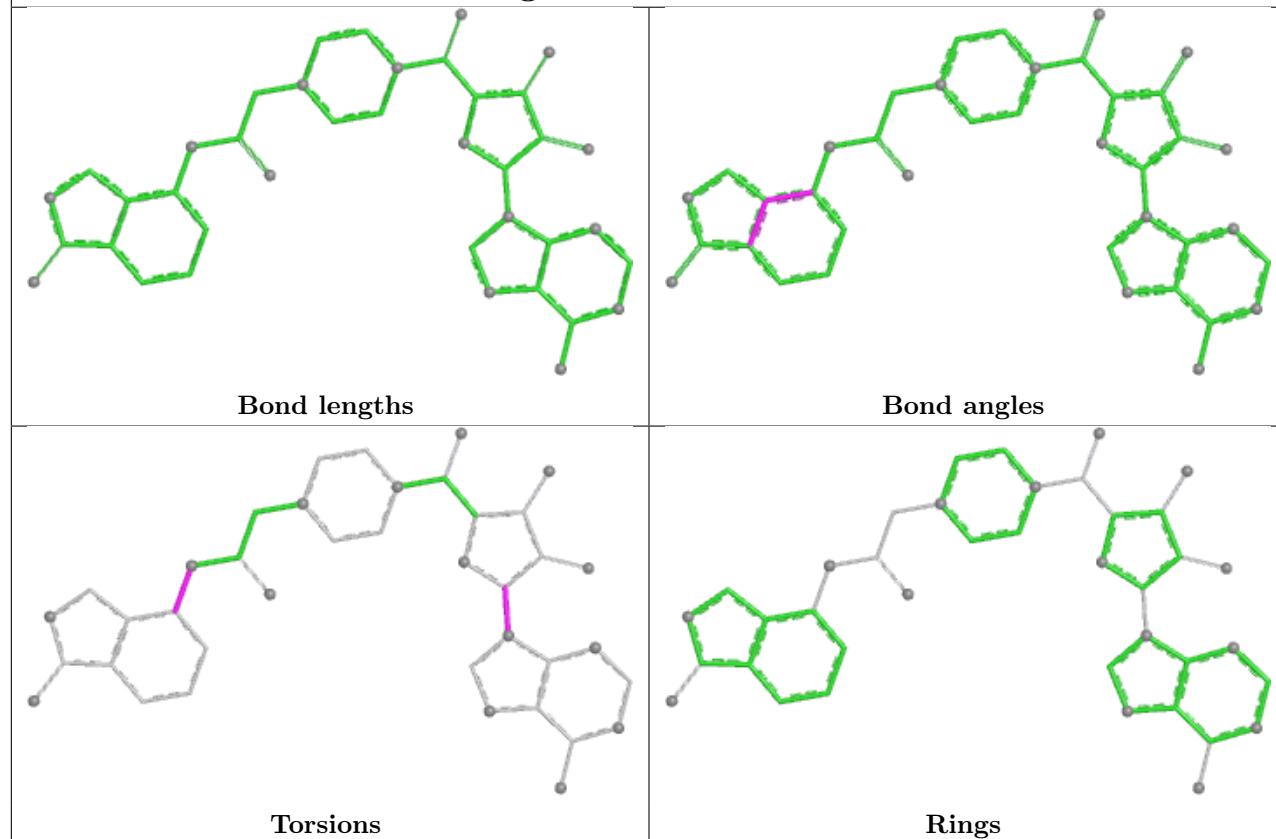
Ligand UHB C 2001



Ligand UHB B 2001



Ligand UHB A 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%)	1.73	124 (36%) 1 0	31, 74, 145, 161	0
1	B	340/372 (91%)	1.77	133 (39%) 1 0	30, 74, 148, 164	0
1	C	340/372 (91%)	1.72	117 (34%) 1 1	29, 71, 152, 165	0
1	D	340/372 (91%)	1.75	127 (37%) 1 0	28, 72, 144, 158	0
All	All	1360/1488 (91%)	1.74	501 (36%) 1 0	28, 73, 148, 165	0

All (501) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	714	SER	7.3
1	C	752	LEU	6.9
1	A	714	SER	6.6
1	C	888	GLY	6.1
1	D	714	SER	6.1
1	A	888	GLY	5.8
1	C	706	ILE	5.7
1	B	963	SER	5.7
1	A	721	SER	5.2
1	A	723	GLY	5.2
1	A	960	ALA	5.2
1	A	706	ILE	5.1
1	B	714	SER	5.1
1	A	963	SER	5.1
1	D	888	GLY	5.1
1	A	766	ASP	5.1
1	A	972	GLY	5.0
1	B	719	ALA	5.0
1	D	706	ILE	4.9
1	B	721	SER	4.9
1	D	963	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	719	ALA	4.8
1	B	958	PRO	4.8
1	C	721	SER	4.8
1	D	752	LEU	4.8
1	A	887	THR	4.7
1	A	818	VAL	4.7
1	D	721	SER	4.7
1	A	713	LEU	4.6
1	B	705	GLN	4.6
1	C	723	GLY	4.6
1	D	948	VAL	4.6
1	C	972	GLY	4.6
1	C	705	GLN	4.6
1	A	957	ASP	4.5
1	D	958	PRO	4.5
1	A	716	VAL	4.5
1	B	888	GLY	4.4
1	C	963	SER	4.4
1	A	861	TRP	4.4
1	B	836	ILE	4.4
1	A	719	ALA	4.4
1	C	957	ASP	4.4
1	D	723	GLY	4.4
1	C	889	TYR	4.4
1	B	899	ASP	4.4
1	D	716	VAL	4.3
1	D	717	GLN	4.3
1	C	958	PRO	4.3
1	D	705	GLN	4.3
1	C	716	VAL	4.3
1	C	948	VAL	4.3
1	B	957	ASP	4.3
1	B	768	LEU	4.3
1	D	713	LEU	4.3
1	C	718	GLN	4.2
1	A	853	GLN	4.2
1	A	768	LEU	4.2
1	B	770	ASP	4.2
1	C	717	GLN	4.2
1	B	948	VAL	4.2
1	A	958	PRO	4.1
1	D	736	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	766	ASP	4.1
1	D	722	GLN	4.1
1	A	899	ASP	4.1
1	A	777	LEU	4.1
1	D	768	LEU	4.1
1	B	717	GLN	4.1
1	B	972	GLY	4.0
1	D	972	GLY	4.0
1	A	752	LEU	4.0
1	C	722	GLN	4.0
1	A	959	SER	4.0
1	B	722	GLN	4.0
1	B	818	VAL	4.0
1	D	887	THR	4.0
1	D	770	ASP	3.9
1	C	736	PHE	3.9
1	B	727	SER	3.9
1	C	960	ALA	3.9
1	D	957	ASP	3.9
1	C	777	LEU	3.9
1	C	727	SER	3.9
1	B	720	VAL	3.8
1	C	853	GLN	3.8
1	B	706	ILE	3.8
1	C	768	LEU	3.8
1	A	886	VAL	3.8
1	A	717	GLN	3.8
1	B	947	SER	3.8
1	D	899	ASP	3.8
1	A	836	ILE	3.8
1	B	777	LEU	3.8
1	B	832	GLU	3.8
1	D	962	ILE	3.8
1	B	853	GLN	3.8
1	A	969	VAL	3.7
1	A	722	GLN	3.7
1	C	770	ASP	3.7
1	D	718	GLN	3.7
1	D	853	GLN	3.7
1	B	752	LEU	3.7
1	B	861	TRP	3.7
1	B	718	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	731	ASP	3.7
1	B	723	GLY	3.7
1	C	959	SER	3.7
1	A	718	GLN	3.7
1	D	823	ALA	3.7
1	D	720	VAL	3.7
1	D	980	ASN	3.6
1	B	716	VAL	3.6
1	B	821	THR	3.6
1	C	887	THR	3.6
1	C	810	GLU	3.6
1	C	836	ILE	3.6
1	A	936	SER	3.6
1	A	736	PHE	3.6
1	D	886	VAL	3.6
1	D	704	ARG	3.6
1	D	891	PHE	3.6
1	B	975	ILE	3.6
1	A	810	GLU	3.6
1	A	948	VAL	3.5
1	B	886	VAL	3.5
1	C	804	VAL	3.5
1	C	962	ILE	3.5
1	A	828	ALA	3.5
1	B	960	ALA	3.5
1	D	832	GLU	3.4
1	B	959	SER	3.4
1	C	947	SER	3.4
1	D	936	SER	3.4
1	A	770	ASP	3.4
1	B	732	LEU	3.4
1	B	704	ARG	3.4
1	C	712	ILE	3.4
1	A	889	TYR	3.4
1	C	766	ASP	3.4
1	D	889	TYR	3.4
1	D	771	ILE	3.4
1	C	899	ASP	3.4
1	B	804	VAL	3.3
1	C	891	PHE	3.3
1	B	736	PHE	3.3
1	B	817	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	938	ILE	3.3
1	C	732	LEU	3.3
1	A	705	GLN	3.3
1	C	773	VAL	3.3
1	D	773	VAL	3.3
1	A	902	SER	3.3
1	C	981	ASP	3.3
1	D	777	LEU	3.3
1	B	936	SER	3.3
1	D	727	SER	3.3
1	B	889	TYR	3.2
1	A	820	ASN	3.2
1	B	962	ILE	3.2
1	D	836	ILE	3.2
1	B	823	ALA	3.2
1	C	886	VAL	3.2
1	C	818	VAL	3.2
1	C	969	VAL	3.2
1	D	967	VAL	3.2
1	D	969	VAL	3.2
1	B	746	MET	3.2
1	B	712	ILE	3.2
1	C	975	ILE	3.2
1	B	766	ASP	3.1
1	B	807	ASP	3.1
1	D	818	VAL	3.1
1	A	821	THR	3.1
1	A	962	ILE	3.1
1	A	724	SER	3.1
1	B	902	SER	3.1
1	A	981	ASP	3.1
1	C	822	HIS	3.1
1	A	804	VAL	3.1
1	B	969	VAL	3.1
1	D	712	ILE	3.1
1	B	735	ARG	3.1
1	A	755	ALA	3.1
1	D	947	SER	3.1
1	D	959	SER	3.1
1	D	821	THR	3.1
1	B	710	TYR	3.1
1	B	937	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	939	SER	3.1
1	C	726	ASP	3.1
1	B	978	GLY	3.1
1	A	790	ILE	3.1
1	D	729	ILE	3.1
1	B	810	GLU	3.1
1	D	804	VAL	3.0
1	B	938	ILE	3.0
1	C	832	GLU	3.0
1	B	887	THR	3.0
1	A	720	VAL	3.0
1	B	822	HIS	3.0
1	B	726	ASP	3.0
1	C	936	SER	3.0
1	A	771	ILE	3.0
1	C	729	ILE	3.0
1	D	755	ALA	3.0
1	D	828	ALA	3.0
1	A	773	VAL	3.0
1	A	891	PHE	3.0
1	D	758	VAL	3.0
1	A	980	ASN	3.0
1	B	980	ASN	3.0
1	B	713	LEU	3.0
1	C	821	THR	3.0
1	D	719	ALA	3.0
1	C	979	VAL	3.0
1	B	775	TYR	3.0
1	D	938	ILE	3.0
1	B	707	GLN	3.0
1	D	941	LEU	3.0
1	C	939	SER	3.0
1	C	823	ALA	3.0
1	D	979	VAL	3.0
1	C	771	ILE	2.9
1	D	978	GLY	2.9
1	B	828	ALA	2.9
1	A	967	VAL	2.9
1	D	744	PHE	2.9
1	A	819	LYS	2.9
1	A	729	ILE	2.9
1	B	790	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	765	LEU	2.9
1	C	713	LEU	2.9
1	D	810	GLU	2.9
1	C	980	ASN	2.9
1	A	975	ILE	2.9
1	A	971	LEU	2.9
1	B	951	LEU	2.9
1	A	832	GLU	2.9
1	A	807	ASP	2.9
1	D	819	LYS	2.9
1	D	902	SER	2.9
1	B	771	ILE	2.9
1	A	823	ALA	2.9
1	B	762	ALA	2.9
1	D	960	ALA	2.9
1	A	727	SER	2.9
1	D	937	HIS	2.9
1	A	817	TYR	2.8
1	A	811	ALA	2.8
1	B	815	ARG	2.8
1	C	704	ARG	2.8
1	D	735	ARG	2.8
1	D	762	ALA	2.8
1	A	822	HIS	2.8
1	A	704	ARG	2.8
1	B	685	ALA	2.8
1	A	733	SER	2.8
1	B	905	ALA	2.8
1	B	819	LYS	2.8
1	D	711	SER	2.8
1	A	974	GLY	2.8
1	D	759	GLN	2.7
1	A	979	VAL	2.7
1	D	992	TYR	2.7
1	C	937	HIS	2.7
1	B	979	VAL	2.7
1	A	860	LEU	2.7
1	C	828	ALA	2.7
1	D	687	VAL	2.7
1	A	712	ILE	2.7
1	D	765	LEU	2.7
1	D	975	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	934	HIS	2.7
1	B	966	GLY	2.7
1	C	978	GLY	2.7
1	A	947	SER	2.7
1	C	941	LEU	2.7
1	D	932	LEU	2.7
1	B	811	ALA	2.7
1	B	891	PHE	2.7
1	C	819	LYS	2.7
1	B	967	VAL	2.7
1	A	941	LEU	2.6
1	B	765	LEU	2.6
1	C	757	SER	2.6
1	C	902	SER	2.6
1	D	944	GLY	2.6
1	B	971	LEU	2.6
1	D	951	LEU	2.6
1	B	990	ILE	2.6
1	B	776	SER	2.6
1	A	937	HIS	2.6
1	B	885	PRO	2.6
1	C	924	VAL	2.6
1	D	1011	THR	2.6
1	B	729	ILE	2.6
1	A	756	ASP	2.6
1	C	800	ASP	2.6
1	A	939	SER	2.6
1	D	808	SER	2.6
1	D	750	PRO	2.6
1	D	817	TYR	2.6
1	A	990	ILE	2.6
1	A	754	ASN	2.6
1	B	754	ASN	2.6
1	A	726	ASP	2.6
1	A	776	SER	2.5
1	D	939	SER	2.5
1	C	861	TRP	2.5
1	A	944	GLY	2.5
1	B	860	LEU	2.5
1	C	815	ARG	2.5
1	D	822	HIS	2.5
1	B	808	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	941	LEU	2.5
1	C	971	LEU	2.5
1	D	915	PRO	2.5
1	D	740	ILE	2.5
1	D	715	GLU	2.5
1	A	808	SER	2.5
1	C	967	VAL	2.5
1	D	754	ASN	2.5
1	B	769	LEU	2.5
1	C	990	ILE	2.5
1	D	892	GLY	2.5
1	B	1007	PHE	2.5
1	A	707	GLN	2.5
1	A	700	LYS	2.5
1	C	961	ASN	2.5
1	D	971	LEU	2.4
1	D	981	ASP	2.4
1	B	894	GLY	2.4
1	B	733	SER	2.4
1	B	976	SER	2.4
1	C	905	ALA	2.4
1	D	689	TYR	2.4
1	B	973	THR	2.4
1	B	981	ASP	2.4
1	D	726	ASP	2.4
1	D	800	ASP	2.4
1	D	885	PRO	2.4
1	B	997	VAL	2.4
1	D	861	TRP	2.4
1	B	691	ILE	2.4
1	C	811	ALA	2.4
1	C	860	LEU	2.4
1	B	919	ILE	2.4
1	B	758	VAL	2.4
1	D	745	GLY	2.4
1	A	815	ARG	2.4
1	A	858	ARG	2.4
1	C	930	TYR	2.4
1	A	691	ILE	2.4
1	B	820	ASN	2.3
1	C	833	VAL	2.3
1	D	671	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	774	ALA	2.3
1	A	746	MET	2.3
1	B	1011	THR	2.3
1	B	745	GLY	2.3
1	A	905	ALA	2.3
1	D	842	GLU	2.3
1	C	728	GLN	2.3
1	A	932	LEU	2.3
1	C	776	SER	2.3
1	C	904	SER	2.3
1	D	977	SER	2.3
1	A	955	THR	2.3
1	A	973	THR	2.3
1	D	710	TYR	2.3
1	D	813	ILE	2.3
1	B	901	VAL	2.3
1	B	991	VAL	2.3
1	A	978	GLY	2.3
1	C	709	ALA	2.3
1	C	756	ASP	2.3
1	A	769	LEU	2.3
1	A	859	LEU	2.3
1	B	806	ARG	2.3
1	C	775	TYR	2.3
1	C	992	TYR	2.3
1	A	991	VAL	2.3
1	A	894	GLY	2.3
1	C	820	ASN	2.3
1	D	820	ASN	2.3
1	B	708	ALA	2.3
1	B	715	GLU	2.3
1	A	778	LEU	2.3
1	B	778	LEU	2.3
1	B	968	ASP	2.3
1	C	759	GLN	2.3
1	B	858	ARG	2.3
1	B	930	TYR	2.3
1	C	710	TYR	2.3
1	A	890	MET	2.2
1	B	728	GLN	2.2
1	C	846	GLN	2.2
1	A	830	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	968	ASP	2.2
1	A	735	ARG	2.2
1	B	824	THR	2.2
1	D	955	THR	2.2
1	D	775	TYR	2.2
1	D	781	GLY	2.2
1	B	840	GLU	2.2
1	C	715	GLU	2.2
1	C	769	LEU	2.2
1	D	700	LYS	2.2
1	B	846	GLN	2.2
1	C	807	ASP	2.2
1	C	914	ASP	2.2
1	D	749	PRO	2.2
1	B	932	LEU	2.2
1	D	732	LEU	2.2
1	D	846	GLN	2.2
1	A	678	ASP	2.2
1	B	756	ASP	2.2
1	C	720	VAL	2.2
1	C	991	VAL	2.2
1	A	904	SER	2.2
1	C	725	SER	2.2
1	B	849	LYS	2.2
1	D	835	ASP	2.2
1	A	992	TYR	2.2
1	C	744	PHE	2.2
1	A	730	LEU	2.2
1	A	873	LEU	2.2
1	C	739	LEU	2.2
1	D	698	LEU	2.2
1	B	988	GLU	2.2
1	C	827	ASN	2.1
1	D	961	ASN	2.1
1	B	900	MET	2.1
1	C	849	LYS	2.1
1	D	894	GLY	2.1
1	C	932	LEU	2.1
1	B	711	SER	2.1
1	C	977	SER	2.1
1	D	733	SER	2.1
1	D	776	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	688	GLU	2.1
1	C	754	ASN	2.1
1	A	687	VAL	2.1
1	C	997	VAL	2.1
1	D	866	THR	2.1
1	C	951	LEU	2.1
1	A	935	ALA	2.1
1	A	919	ILE	2.1
1	D	707	GLN	2.1
1	D	728	GLN	2.1
1	A	833	VAL	2.1
1	A	924	VAL	2.1
1	B	833	VAL	2.1
1	D	901	VAL	2.1
1	C	894	GLY	2.1
1	A	938	ILE	2.1
1	B	755	ALA	2.1
1	A	874	SER	2.1
1	C	976	SER	2.1
1	D	911	SER	2.1
1	C	670	GLN	2.1
1	B	761	LYS	2.1
1	A	831	LEU	2.1
1	A	824	THR	2.1
1	B	993	ASP	2.1
1	C	755	ALA	2.1
1	D	685	ALA	2.1
1	D	905	ALA	2.1
1	A	715	GLU	2.1
1	B	842	GLU	2.1
1	C	840	GLU	2.1
1	B	848	TYR	2.1
1	C	724	SER	2.0
1	A	997	VAL	2.0
1	A	961	ASN	2.0
1	A	950	GLY	2.0
1	D	691	ILE	2.0
1	D	990	ILE	2.0
1	A	685	ALA	2.0
1	A	710	TYR	2.0
1	C	700	LYS	2.0
1	C	761	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	829	TYR	2.0
1	A	759	GLN	2.0
1	D	904	SER	2.0
1	D	1005	LEU	2.0
1	D	815	ARG	2.0
1	A	744	PHE	2.0
1	A	781	GLY	2.0
1	B	892	GLY	2.0
1	B	944	GLY	2.0
1	D	699	GLY	2.0
1	B	935	ALA	2.0
1	C	955	THR	2.0
1	C	731	ASP	2.0
1	B	748	LYS	2.0
1	C	988	GLU	2.0
1	A	930	TYR	2.0
1	C	758	VAL	2.0
1	D	924	VAL	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	UHB	A	2001	39/39	0.73	0.16	49,77,83,83	0
2	UHB	B	2001	39/39	0.73	0.17	51,81,88,88	0
3	SO4	B	2004	5/5	0.76	0.15	56,60,62,65	0
2	UHB	D	2001	39/39	0.77	0.17	43,76,86,86	0
3	SO4	C	2004	5/5	0.77	0.14	57,58,63,63	0

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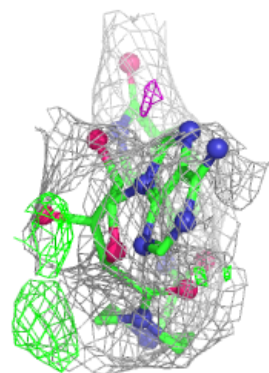
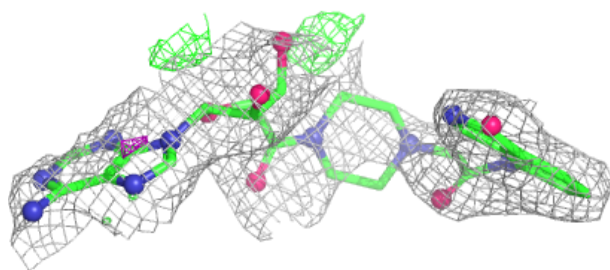
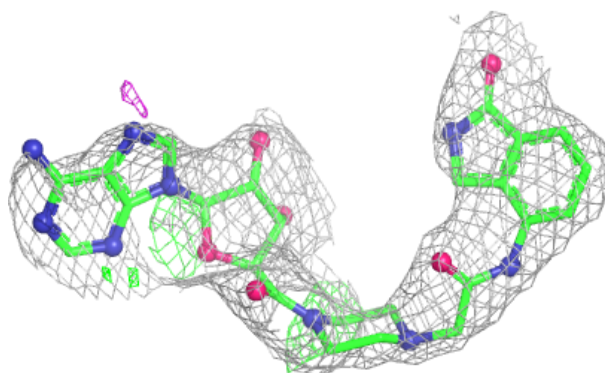
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	D	2004	5/5	0.77	0.16	55,58,62,63	0
2	UHB	C	2001	39/39	0.78	0.15	38,74,81,82	0
3	SO4	B	2003	5/5	0.80	0.20	73,75,78,78	0
3	SO4	A	2003	5/5	0.81	0.17	67,69,72,74	0
3	SO4	C	2003	5/5	0.83	0.19	67,67,69,71	0
3	SO4	C	2002	5/5	0.84	0.18	77,77,79,81	0
3	SO4	D	2002	5/5	0.84	0.16	75,76,80,80	0
3	SO4	D	2003	5/5	0.84	0.20	65,65,67,68	0
3	SO4	A	2002	5/5	0.84	0.16	77,78,80,83	0
3	SO4	A	2004	5/5	0.86	0.14	57,62,62,63	0
3	SO4	B	2002	5/5	0.87	0.14	74,74,76,79	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.

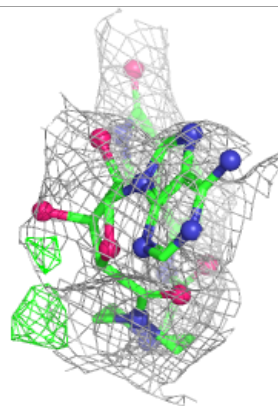
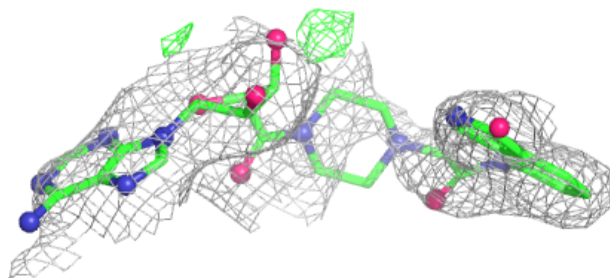
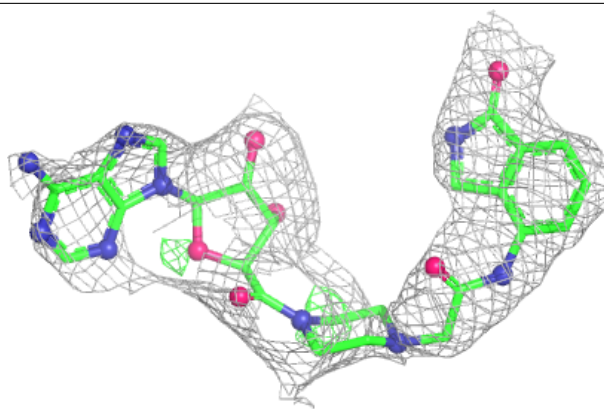
Electron density around UHB A 2001:

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

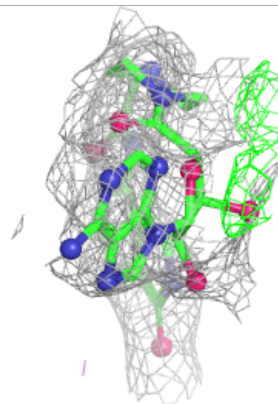
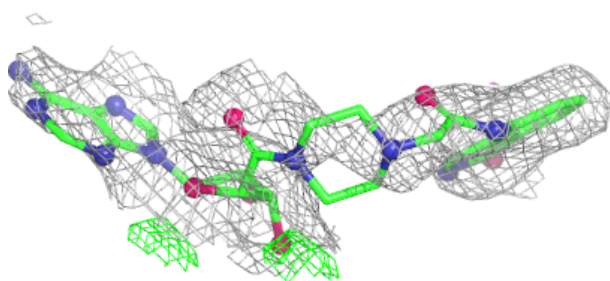
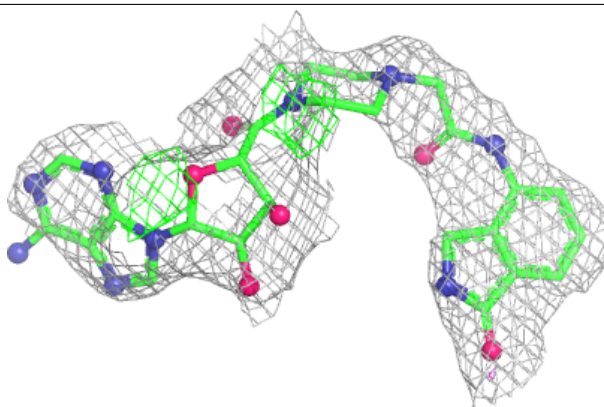


Electron density around UHB B 2001:

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

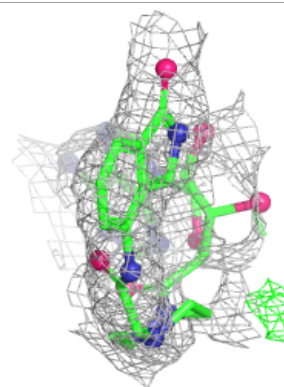
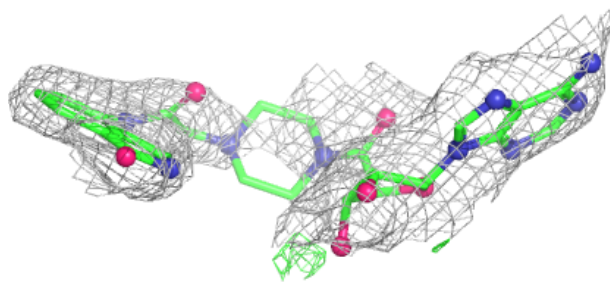
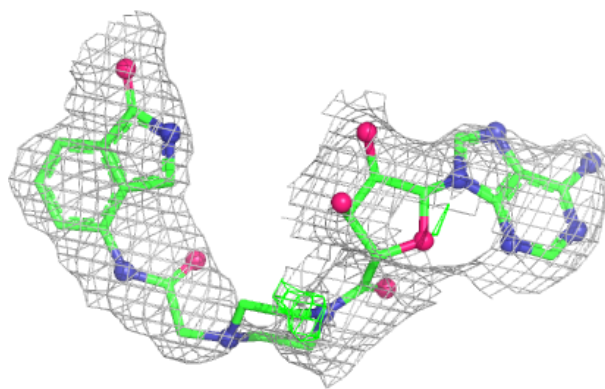
**Electron density around UHB D 2001:**

$2mF_o-DF_c$ (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.