



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:57 AM UTC

PDB ID : 1P17 / pdb_00001p17
Title : Hypoxanthine Phosphoribosyltransferase from Trypanosoma cruzi, K68R mutant, complexed with the product IMP
Authors : Medrano, F.J.; Eakin, A.E.; Craig III, S.P.
Deposited on : 2003-04-11
Resolution : 2.70 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

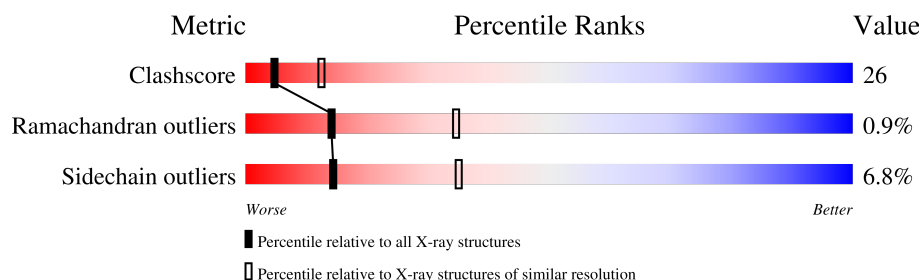
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	
1	B	221	
1	C	221	
1	D	221	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6768 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.

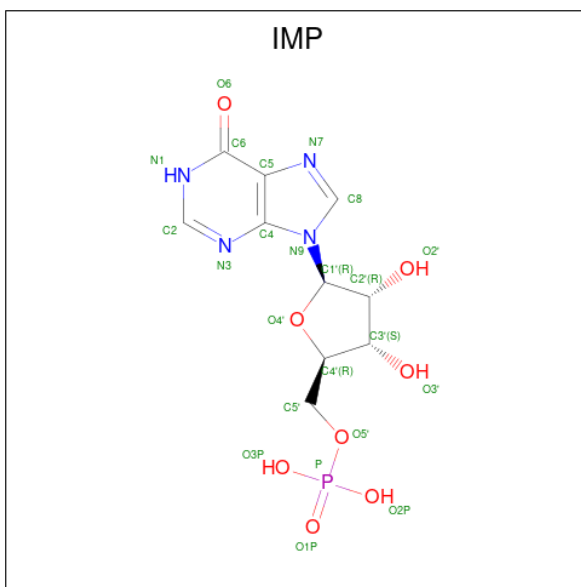
- Molecule 1 is a protein called hypoxanthine phosphoribosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1573	1006	274	287	6			
1	B	204	Total	C	N	O	S	0	0	0
			1649	1051	291	301	6			
1	C	192	Total	C	N	O	S	0	0	0
			1555	996	269	284	6			
1	D	188	Total	C	N	O	S	0	0	0
			1539	987	268	278	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LYS	MET	SEE REMARK 999	UNP Q27796
A	52	ARG	LYS	engineered mutation	UNP Q27796
A	66	CYS	SER	SEE REMARK 999	UNP Q27796
A	86	LEU	VAL	SEE REMARK 999	UNP Q27796
B	23	LYS	MET	SEE REMARK 999	UNP Q27796
B	52	ARG	LYS	engineered mutation	UNP Q27796
B	66	CYS	SER	SEE REMARK 999	UNP Q27796
B	86	LEU	VAL	SEE REMARK 999	UNP Q27796
C	23	LYS	MET	SEE REMARK 999	UNP Q27796
C	52	ARG	LYS	engineered mutation	UNP Q27796
C	66	CYS	SER	SEE REMARK 999	UNP Q27796
C	86	LEU	VAL	SEE REMARK 999	UNP Q27796
D	23	LYS	MET	SEE REMARK 999	UNP Q27796
D	52	ARG	LYS	engineered mutation	UNP Q27796
D	66	CYS	SER	SEE REMARK 999	UNP Q27796
D	86	LEU	VAL	SEE REMARK 999	UNP Q27796

- Molecule 2 is INOSINIC ACID (CCD ID: IMP) (formula: C₁₀H₁₃N₄O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is water.

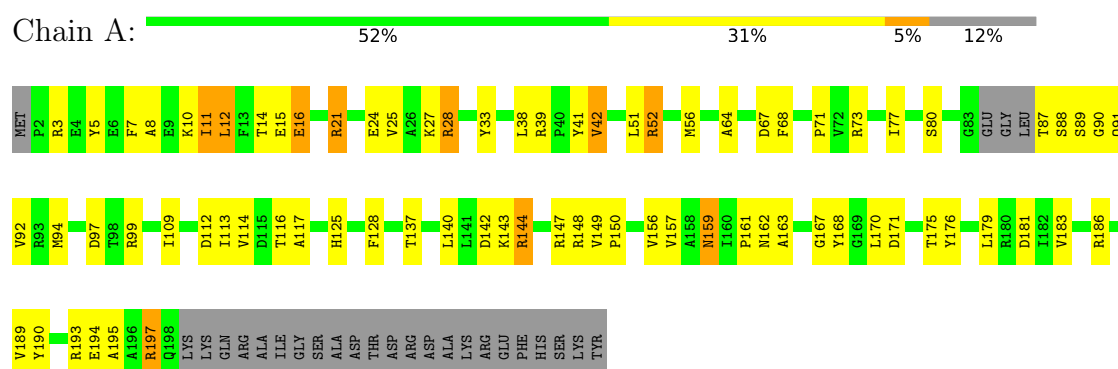
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	105	Total	O	0	0
			105	105		
3	B	119	Total	O	0	0
			119	119		
3	C	60	Total	O	0	0
			60	60		
3	D	76	Total	O	0	0
			76	76		

3 Residue-property plots

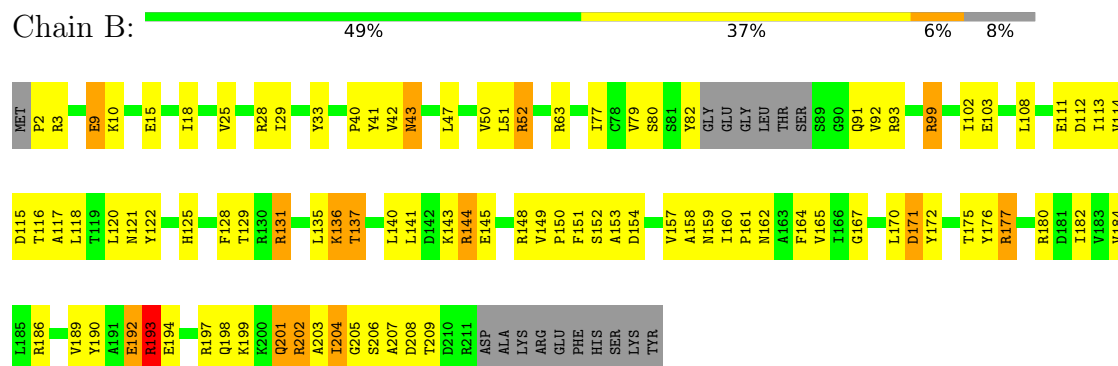
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

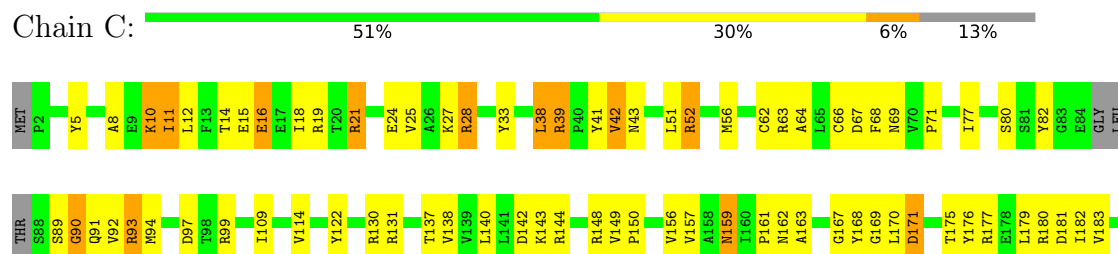
- Molecule 1: hypoxanthine phosphoribosyltransferase

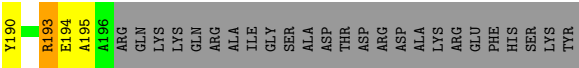


- Molecule 1: hypoxanthine phosphoribosyltransferase

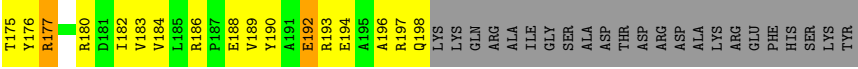
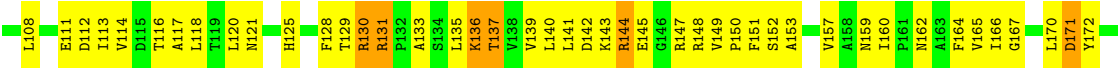
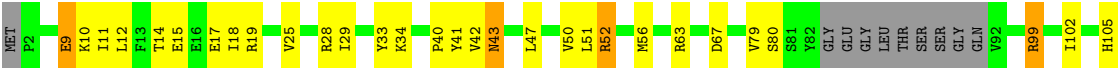


- Molecule 1: hypoxanthine phosphoribosyltransferase





● Molecule 1: hypoxanthine phosphoribosyltransferase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.31Å 122.88Å 52.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.70)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6768	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.52	0/1604	0.99	8/2171 (0.4%)
1	B	0.51	0/1680	0.98	9/2270 (0.4%)
1	C	0.49	0/1586	1.01	8/2147 (0.4%)
1	D	0.50	0/1570	0.98	7/2125 (0.3%)
All	All	0.50	0/6440	0.99	32/8713 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	ASP	N-CA-C	7.49	119.07	108.74
1	C	39	ARG	NE-CZ-NH2	7.42	125.88	119.20
1	B	148	ARG	N-CA-C	-7.35	103.91	114.12
1	B	171	ASP	N-CA-C	7.35	118.88	108.74
1	C	42	VAL	N-CA-C	7.09	117.88	110.72
1	A	42	VAL	N-CA-C	6.93	117.72	110.72
1	D	148	ARG	N-CA-C	-6.87	104.57	114.12
1	C	131	ARG	CA-C-N	-6.19	114.27	120.21
1	C	131	ARG	C-N-CA	-6.19	114.27	120.21
1	D	42	VAL	N-CA-C	6.16	117.11	111.81
1	B	42	VAL	N-CA-C	6.00	116.97	111.81
1	D	50	VAL	N-CA-C	5.94	115.81	107.37
1	B	131	ARG	CB-CA-C	-5.76	107.11	111.20
1	A	171	ASP	N-CA-C	5.75	117.34	109.18
1	D	131	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	A	195	ALA	N-CA-C	-5.59	98.90	110.80
1	A	88	SER	N-CA-C	-5.58	106.36	112.72
1	A	197	ARG	N-CA-C	-5.57	101.20	109.83
1	C	195	ALA	N-CA-C	5.55	118.27	109.50
1	B	102	ILE	N-CA-C	-5.41	107.54	113.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	102	ILE	N-CA-C	-5.38	107.57	113.43
1	B	193	ARG	NE-CZ-NH2	5.36	124.02	119.20
1	D	131	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	A	144	ARG	NE-CZ-NH1	-5.24	116.26	121.50
1	A	144	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	A	144	ARG	N-CA-C	5.19	117.67	111.71
1	B	3	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	C	63	ARG	N-CA-C	-5.11	105.60	111.07
1	C	90	GLY	N-CA-C	-5.07	108.98	115.42
1	B	148	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	B	177	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	C	171	ASP	N-CA-C	5.02	116.31	109.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1573	0	1570	82	0
1	B	1649	0	1650	106	1
1	C	1555	0	1550	82	0
1	D	1539	0	1538	92	0
2	A	23	0	11	1	0
2	B	23	0	11	0	0
2	C	23	0	11	1	0
2	D	23	0	11	1	0
3	A	105	0	0	6	0
3	B	119	0	0	12	0
3	C	60	0	0	3	0
3	D	76	0	0	6	0
All	All	6768	0	6352	327	1

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 26.

All (327) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.11	1.08
1:C:28:ARG:HG2	1:C:28:ARG:HH11	1.24	0.99
1:C:33:TYR:HB3	1:C:38:LEU:HD21	1.55	0.89
1:B:171:ASP:OD2	1:B:177:ARG:NH1	2.06	0.89
1:A:109:ILE:HB	1:A:137:THR:HG22	1.56	0.87
1:A:193:ARG:HH21	1:B:41:TYR:HB3	1.39	0.86
1:A:28:ARG:HG2	1:A:28:ARG:NH1	1.87	0.85
1:C:144:ARG:HD2	1:C:159:ASN:HD21	1.41	0.85
1:B:2:PRO:HG2	3:B:3055:HOH:O	1.79	0.83
1:C:41:TYR:CB	1:D:193:ARG:HH21	1.90	0.83
1:A:33:TYR:HB3	1:A:38:LEU:HD21	1.60	0.82
1:A:28:ARG:HH11	1:A:28:ARG:CG	1.93	0.81
1:C:28:ARG:HH11	1:C:28:ARG:CG	1.93	0.81
1:C:99:ARG:HD3	1:D:52:ARG:NH2	1.95	0.80
1:C:109:ILE:HB	1:C:137:THR:HG22	1.66	0.78
1:C:19:ARG:HG3	1:C:19:ARG:HH21	1.47	0.78
1:D:171:ASP:OD2	1:D:177:ARG:NH1	2.21	0.73
1:A:144:ARG:HD3	1:A:159:ASN:HD21	1.54	0.72
1:A:193:ARG:NH2	1:B:41:TYR:HB3	2.04	0.72
1:A:38:LEU:HB3	1:A:71:PRO:HG2	1.71	0.71
1:C:38:LEU:HB3	1:C:71:PRO:HG2	1.73	0.70
1:B:144:ARG:HD3	1:B:159:ASN:HD22	1.58	0.69
1:B:9:GLU:HG2	1:B:10:LYS:HG2	1.75	0.68
1:C:90:GLY:O	1:C:92:VAL:HG13	1.93	0.68
1:D:190:TYR:CE1	1:D:194:GLU:HG3	2.29	0.68
1:C:193:ARG:HH21	1:D:41:TYR:HB3	1.58	0.68
1:B:52:ARG:NH2	3:B:3074:HOH:O	2.27	0.68
1:D:171:ASP:HB3	1:D:177:ARG:HH11	1.58	0.68
1:C:66:CYS:HA	3:C:3019:HOH:O	1.94	0.68
1:B:125:HIS:O	1:B:129:THR:HG23	1.94	0.67
1:B:208:ASP:HB2	1:C:190:TYR:OH	1.95	0.67
1:D:177:ARG:HH11	1:D:177:ARG:CG	2.08	0.67
1:B:143:LYS:O	1:B:145:GLU:N	2.28	0.67
1:A:41:TYR:CE2	1:B:193:ARG:HD3	2.29	0.66
1:B:201:GLN:HG2	1:B:202:ARG:N	2.11	0.66
1:A:11:ILE:N	1:A:11:ILE:HD12	2.10	0.66
1:A:5:TYR:HB2	1:A:8:ALA:HB3	1.77	0.65
1:B:172:TYR:HE2	1:B:193:ARG:HG2	1.61	0.65
1:C:5:TYR:HB2	1:C:8:ALA:HB3	1.78	0.65
1:C:193:ARG:NH2	1:D:41:TYR:HB3	2.12	0.65
1:C:94:MET:HE1	1:C:97:ASP:HA	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:HG22	1:A:90:GLY:H	1.61	0.65
1:A:15:GLU:HB3	1:A:16:GLU:OE1	1.97	0.65
1:D:143:LYS:O	1:D:145:GLU:N	2.29	0.65
1:B:190:TYR:CE1	1:B:194:GLU:HG3	2.32	0.64
1:D:171:ASP:HB3	1:D:177:ARG:NH1	2.12	0.64
1:B:205:GLY:O	1:B:207:ALA:N	2.30	0.64
1:A:140:LEU:HD21	1:A:168:TYR:HD2	1.61	0.64
1:D:144:ARG:HD3	1:D:159:ASN:HD22	1.62	0.64
1:D:9:GLU:HG2	1:D:10:LYS:HG2	1.80	0.64
1:C:21:ARG:O	1:C:25:VAL:HG23	1.98	0.63
1:D:113:ILE:HD11	1:D:143:LYS:HE3	1.79	0.63
1:D:28:ARG:NH2	3:D:3067:HOH:O	2.32	0.63
1:C:16:GLU:N	1:C:16:GLU:OE1	2.32	0.63
1:A:94:MET:HE1	1:A:97:ASP:HA	1.81	0.62
1:D:177:ARG:HH11	1:D:177:ARG:HG2	1.64	0.62
1:D:125:HIS:O	1:D:129:THR:HG23	2.00	0.62
1:A:190:TYR:O	1:A:194:GLU:HG2	2.00	0.62
1:C:28:ARG:HG2	1:C:28:ARG:NH1	1.98	0.62
1:B:144:ARG:HD3	1:B:159:ASN:ND2	2.15	0.62
1:A:51:LEU:HD11	1:B:51:LEU:HD11	1.80	0.61
1:B:103:GLU:OE2	1:B:131:ARG:NH1	2.33	0.61
1:D:167:GLY:HA2	1:D:176:TYR:O	2.00	0.61
1:C:11:ILE:N	1:C:11:ILE:HD12	2.16	0.61
1:C:51:LEU:HD11	1:D:51:LEU:HD11	1.83	0.61
1:C:140:LEU:HD21	1:C:168:TYR:HD2	1.67	0.60
1:B:113:ILE:HD11	1:B:143:LYS:HE3	1.82	0.60
1:D:10:LYS:HD3	3:D:3043:HOH:O	2.00	0.60
1:A:149:VAL:HG23	1:A:150:PRO:HD2	1.84	0.60
1:A:99:ARG:HD3	1:B:52:ARG:HH22	1.66	0.60
1:A:21:ARG:O	1:A:25:VAL:HG23	2.02	0.59
1:C:99:ARG:HD3	1:D:52:ARG:HH21	1.66	0.59
1:B:141:LEU:HD12	1:B:170:LEU:HD11	1.82	0.59
1:C:15:GLU:HB3	1:C:16:GLU:OE1	2.01	0.59
1:A:41:TYR:CZ	1:B:193:ARG:HD3	2.37	0.59
1:B:161:PRO:HD3	3:B:3054:HOH:O	2.02	0.59
1:C:144:ARG:HD2	1:C:159:ASN:ND2	2.16	0.59
1:A:56:MET:CE	1:B:63:ARG:HG3	2.33	0.58
1:B:18:ILE:HD11	1:B:182:ILE:HG13	1.85	0.58
1:B:43:ASN:C	1:B:43:ASN:HD22	2.11	0.58
1:C:190:TYR:O	1:C:194:GLU:HG2	2.03	0.58
3:A:3094:HOH:O	1:C:99:ARG:HD2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:HG3	3:A:3053:HOH:O	2.04	0.57
1:B:9:GLU:HA	3:B:3071:HOH:O	2.03	0.57
1:C:38:LEU:HB3	1:C:71:PRO:CG	2.34	0.57
1:C:143:LYS:NZ	2:C:3002:IMP:O6	2.37	0.57
1:B:92:VAL:HG13	1:B:122:TYR:CE2	2.40	0.57
1:C:149:VAL:HG23	1:C:150:PRO:HD2	1.87	0.57
1:B:79:VAL:HG11	1:B:91:GLN:O	2.05	0.56
1:A:113:ILE:HD13	2:A:3000:IMP:N7	2.19	0.56
1:C:114:VAL:O	1:C:114:VAL:HG13	2.05	0.56
1:D:144:ARG:HD3	1:D:159:ASN:ND2	2.21	0.56
1:B:114:VAL:HB	1:B:120:LEU:HD12	1.88	0.56
1:D:43:ASN:C	1:D:43:ASN:HD22	2.13	0.56
1:C:41:TYR:HB2	1:D:193:ARG:HH21	1.71	0.56
1:D:197:ARG:O	1:D:198:GLN:HG3	2.04	0.55
1:A:197:ARG:O	1:A:197:ARG:HG3	2.06	0.55
1:B:47:LEU:CD2	1:B:108:LEU:HD23	2.37	0.55
1:B:207:ALA:O	1:B:209:THR:HG23	2.07	0.55
1:C:144:ARG:CD	1:C:159:ASN:HD21	2.17	0.54
1:B:47:LEU:HD23	1:B:108:LEU:HB3	1.89	0.54
1:B:167:GLY:HA2	1:B:176:TYR:O	2.07	0.54
1:B:193:ARG:HE	1:B:193:ARG:HA	1.71	0.54
1:C:69:ASN:HB2	3:C:3049:HOH:O	2.08	0.54
1:D:114:VAL:HB	1:D:120:LEU:HD12	1.89	0.54
1:B:149:VAL:HG22	3:B:3030:HOH:O	2.08	0.54
1:C:56:MET:CE	1:D:63:ARG:HG3	2.37	0.54
1:D:190:TYR:HE1	1:D:194:GLU:HG3	1.71	0.54
1:C:161:PRO:O	1:C:163:ALA:N	2.39	0.53
1:D:149:VAL:CG2	1:D:150:PRO:HD2	2.39	0.53
1:D:190:TYR:CD1	1:D:194:GLU:HG3	2.43	0.53
1:C:170:LEU:N	1:C:170:LEU:HD12	2.23	0.53
1:D:171:ASP:C	1:D:171:ASP:OD1	2.52	0.53
1:D:189:VAL:O	1:D:193:ARG:HB2	2.08	0.53
1:A:114:VAL:HG13	1:A:114:VAL:O	2.07	0.53
1:D:116:THR:O	1:D:117:ALA:HB3	2.08	0.53
1:B:202:ARG:O	1:B:204:ILE:HG13	2.08	0.53
1:D:33:TYR:OH	1:D:136:LYS:HE3	2.08	0.53
1:C:170:LEU:HD12	1:C:170:LEU:H	1.73	0.53
1:B:190:TYR:CD1	1:B:194:GLU:HG3	2.43	0.53
1:D:141:LEU:HD12	1:D:170:LEU:HD11	1.90	0.53
1:C:169:GLY:O	1:C:177:ARG:HG2	2.10	0.52
1:D:47:LEU:HD23	1:D:108:LEU:HB3	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:CG2	1:A:150:PRO:HD2	2.39	0.52
1:C:148:ARG:HH11	1:C:148:ARG:HG2	1.74	0.52
1:D:111:GLU:HG3	1:D:120:LEU:HG	1.91	0.52
1:B:165:VAL:HG23	1:B:170:LEU:HD13	1.92	0.52
1:B:171:ASP:OD1	1:B:171:ASP:C	2.52	0.52
1:B:111:GLU:HG3	1:B:120:LEU:HG	1.91	0.52
1:B:136:LYS:HG3	1:B:154:ASP:CG	2.35	0.52
1:B:172:TYR:CE2	1:B:193:ARG:HG2	2.45	0.52
1:D:165:VAL:HG23	1:D:170:LEU:HD13	1.92	0.51
1:D:112:ASP:O	1:D:140:LEU:HB3	2.09	0.51
1:A:38:LEU:HB3	1:A:71:PRO:CG	2.39	0.51
1:A:148:ARG:HG2	1:A:148:ARG:HH11	1.76	0.51
1:B:140:LEU:O	1:B:157:VAL:HB	2.10	0.51
1:C:41:TYR:HB3	1:D:193:ARG:HH21	1.74	0.51
1:B:2:PRO:HG3	3:B:3022:HOH:O	2.11	0.51
1:B:92:VAL:HG12	1:B:92:VAL:O	2.11	0.51
1:B:112:ASP:O	1:B:140:LEU:HB3	2.11	0.51
1:A:16:GLU:OE1	1:A:16:GLU:N	2.44	0.50
1:A:56:MET:HE2	1:B:63:ARG:HG3	1.92	0.50
1:A:170:LEU:N	1:A:170:LEU:HD12	2.25	0.50
1:B:171:ASP:OD2	1:B:177:ARG:CZ	2.60	0.50
1:C:33:TYR:HB3	1:C:38:LEU:CD2	2.33	0.50
1:C:149:VAL:CG2	1:C:150:PRO:HD2	2.41	0.50
1:D:34:LYS:HD2	3:D:3054:HOH:O	2.10	0.50
1:C:5:TYR:CD1	1:C:183:VAL:HG11	2.47	0.49
1:C:142:ASP:OD1	1:C:143:LYS:N	2.45	0.49
1:A:175:THR:HG22	1:A:176:TYR:N	2.26	0.49
1:C:92:VAL:HG22	1:C:122:TYR:CD2	2.48	0.49
1:A:41:TYR:CB	1:B:193:ARG:NH2	2.76	0.49
1:C:14:THR:HA	1:C:181:ASP:OD1	2.12	0.49
1:A:91:GLN:NE2	1:C:130:ARG:HD3	2.27	0.49
1:C:18:ILE:HD11	1:C:182:ILE:HG13	1.95	0.49
1:B:25:VAL:O	1:B:29:ILE:HG13	2.12	0.48
1:A:41:TYR:CD2	1:B:193:ARG:HD3	2.48	0.48
1:B:192:GLU:O	1:B:192:GLU:HG3	2.13	0.48
1:D:164:PHE:HE2	1:D:172:TYR:HB2	1.78	0.48
1:B:43:ASN:O	1:B:43:ASN:ND2	2.42	0.48
1:B:203:ALA:O	1:B:205:GLY:N	2.46	0.48
1:C:89:SER:C	1:C:91:GLN:H	2.20	0.48
1:D:18:ILE:HD11	1:D:182:ILE:HG13	1.95	0.48
1:A:14:THR:HA	1:A:181:ASP:OD1	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ARG:HG3	1:D:177:ARG:HH21	1.78	0.48
1:A:3:ARG:HD2	1:A:5:TYR:OH	2.14	0.47
1:A:161:PRO:O	1:A:163:ALA:N	2.40	0.47
1:B:51:LEU:HA	1:B:52:ARG:HA	1.71	0.47
1:D:193:ARG:HA	1:D:193:ARG:HD2	1.38	0.47
1:A:170:LEU:HD12	1:A:170:LEU:H	1.79	0.47
1:A:193:ARG:HG2	3:A:3084:HOH:O	2.14	0.47
1:B:149:VAL:CG2	1:B:150:PRO:HD2	2.44	0.47
1:D:19:ARG:HH11	1:D:19:ARG:HG3	1.78	0.47
1:A:27:LYS:HD2	1:A:68:PHE:CE2	2.50	0.47
1:B:190:TYR:O	1:B:190:TYR:HD1	1.97	0.47
1:D:142:ASP:CG	1:D:147:ARG:HH22	2.22	0.47
1:B:190:TYR:HE1	1:B:194:GLU:HG3	1.76	0.47
1:C:80:SER:OG	1:D:99:ARG:NH1	2.47	0.47
1:A:5:TYR:CD1	1:A:183:VAL:HG11	2.49	0.47
1:B:92:VAL:HG13	1:B:122:TYR:CZ	2.49	0.47
1:A:33:TYR:HB3	1:A:38:LEU:CD2	2.39	0.47
1:C:10:LYS:HE3	3:C:3060:HOH:O	2.14	0.47
1:C:62:CYS:SG	1:D:56:MET:HE1	2.54	0.47
1:C:140:LEU:O	1:C:157:VAL:HB	2.14	0.47
1:C:140:LEU:CD2	1:C:168:TYR:HD2	2.27	0.47
1:D:10:LYS:HG2	1:D:184:VAL:CG1	2.44	0.47
1:B:162:ASN:HB3	3:B:3021:HOH:O	2.14	0.47
1:D:141:LEU:HD13	1:D:160:ILE:HD13	1.96	0.47
1:A:77:ILE:HG13	1:A:77:ILE:O	2.14	0.47
1:A:194:GLU:OE1	1:A:194:GLU:HA	2.15	0.47
1:D:192:GLU:O	1:D:192:GLU:HG3	2.14	0.47
1:A:186:ARG:HG3	1:A:189:VAL:HG23	1.97	0.46
1:D:171:ASP:HB3	1:D:177:ARG:HG3	1.96	0.46
1:D:172:TYR:OH	1:D:193:ARG:HB3	2.15	0.46
1:B:40:PRO:O	1:B:41:TYR:HB2	2.15	0.46
1:B:118:LEU:HD22	1:D:131:ARG:HH22	1.80	0.46
1:A:140:LEU:O	1:A:157:VAL:HB	2.15	0.46
1:D:40:PRO:O	1:D:41:TYR:HB2	2.15	0.46
1:D:79:VAL:HG12	1:D:80:SER:N	2.31	0.46
1:B:164:PHE:HE2	1:B:172:TYR:HB2	1.80	0.46
1:D:25:VAL:O	1:D:29:ILE:HG13	2.16	0.46
1:A:167:GLY:CA	1:A:179:LEU:HB2	2.45	0.46
1:B:79:VAL:HG12	1:B:80:SER:N	2.31	0.46
1:D:47:LEU:CD2	1:D:108:LEU:HD23	2.46	0.46
1:D:105:HIS:O	1:D:133:ALA:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:GLU:HB3	3:D:3042:HOH:O	2.15	0.46
1:B:33:TYR:OH	1:B:136:LYS:HE3	2.17	0.45
1:B:144:ARG:CD	3:B:3116:HOH:O	2.64	0.45
1:B:190:TYR:CD1	1:B:190:TYR:C	2.95	0.45
1:C:175:THR:HG22	1:C:176:TYR:N	2.30	0.45
1:C:56:MET:HE1	1:D:63:ARG:HG3	1.98	0.45
1:C:171:ASP:HB3	1:C:177:ARG:CG	2.46	0.45
1:C:171:ASP:HB3	1:C:177:ARG:HG3	1.98	0.45
1:D:140:LEU:O	1:D:157:VAL:HB	2.17	0.45
1:D:196:ALA:HB2	3:D:3073:HOH:O	2.16	0.45
1:A:99:ARG:HD3	1:B:52:ARG:NH2	2.30	0.45
1:D:149:VAL:HG22	1:D:150:PRO:HD2	1.99	0.45
1:A:41:TYR:CG	1:B:193:ARG:NH2	2.75	0.45
1:C:27:LYS:CD	1:C:68:PHE:CE2	2.99	0.45
1:A:64:ALA:HA	1:A:67:ASP:OD2	2.16	0.45
1:A:112:ASP:O	1:A:140:LEU:HB3	2.17	0.45
1:B:120:LEU:HD13	1:B:151:PHE:CE2	2.51	0.45
1:D:166:ILE:HD12	1:D:176:TYR:CD1	2.52	0.45
1:A:11:ILE:N	1:A:11:ILE:CD1	2.78	0.45
1:A:94:MET:CE	1:A:97:ASP:HA	2.46	0.45
1:A:140:LEU:CD2	1:A:168:TYR:HD2	2.28	0.45
1:B:175:THR:HG22	1:B:176:TYR:CD2	2.52	0.45
1:B:189:VAL:O	1:B:193:ARG:HB2	2.16	0.44
1:D:51:LEU:HA	1:D:52:ARG:HA	1.59	0.44
1:D:128:PHE:HB2	1:D:135:LEU:HD23	2.00	0.44
1:B:79:VAL:CG1	1:B:91:GLN:O	2.65	0.44
1:C:21:ARG:NH2	1:C:25:VAL:HG22	2.32	0.44
1:B:201:GLN:C	1:B:203:ALA:H	2.25	0.44
1:C:27:LYS:HD2	1:C:68:PHE:CE2	2.52	0.44
1:D:190:TYR:CD1	1:D:190:TYR:C	2.95	0.44
1:A:21:ARG:HA	1:A:21:ARG:HD2	1.70	0.44
1:A:140:LEU:HD21	1:A:168:TYR:CD2	2.48	0.44
1:A:156:VAL:HG13	1:A:156:VAL:O	2.16	0.44
1:B:15:GLU:OE1	1:B:180:ARG:HB3	2.17	0.44
1:B:190:TYR:HD1	1:B:190:TYR:C	2.25	0.44
1:A:142:ASP:OD1	1:A:143:LYS:N	2.50	0.44
1:B:9:GLU:HG2	1:B:184:VAL:CG1	2.48	0.44
1:C:51:LEU:HA	1:C:52:ARG:HA	1.71	0.44
1:A:125:HIS:O	1:A:128:PHE:HB3	2.17	0.44
1:C:64:ALA:HA	1:C:67:ASP:OD2	2.17	0.44
1:A:167:GLY:HA2	1:A:179:LEU: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:21:ARG:HH21	1:C:25:VAL:CG2	2.31	0.44
1:A:99:ARG:NH2	3:B:3074:HOH:O	2.51	0.44
1:D:99:ARG:HD3	1:D:99:ARG:HA	1.75	0.44
1:A:73:ARG:CG	3:A:3053:HOH:O	2.64	0.44
1:C:94:MET:CE	1:C:97:ASP:HA	2.47	0.44
1:C:167:GLY:CA	1:C:179:LEU:HB2	2.48	0.43
1:B:10:LYS:HG2	1:B:184:VAL:CG1	2.49	0.43
1:B:144:ARG:HD2	3:B:3116:HOH:O	2.17	0.43
1:C:156:VAL:HG13	1:C:156:VAL:O	2.17	0.43
1:D:43:ASN:O	1:D:43:ASN:ND2	2.45	0.43
1:D:186:ARG:C	1:D:188:GLU:N	2.75	0.43
1:A:147:ARG:HG2	1:A:147:ARG:HH11	1.83	0.43
1:B:149:VAL:HG22	1:B:150:PRO:HD2	2.00	0.43
1:A:90:GLY:O	1:A:92:VAL:HG13	2.18	0.43
1:C:90:GLY:O	1:C:91:GLN:C	2.61	0.43
1:D:175:THR:HG22	1:D:176:TYR:CD2	2.54	0.43
1:C:43:ASN:O	1:C:43:ASN:CG	2.61	0.43
1:D:137:THR:HB	3:D:3044:HOH:O	2.18	0.43
1:A:41:TYR:CZ	1:B:193:ARG:CD	3.02	0.43
1:B:141:LEU:HD13	1:B:160:ILE:HD13	2.01	0.43
1:C:180:ARG:HE	1:D:67:ASP:CG	2.27	0.43
1:D:190:TYR:HD1	1:D:190:TYR:O	2.02	0.43
1:A:12:LEU:HD23	3:A:3020:HOH:O	2.19	0.43
1:B:117:ALA:HB1	1:B:151:PHE:HB3	2.01	0.43
1:B:158:ALA:HA	3:B:3033:HOH:O	2.19	0.43
1:D:190:TYR:C	1:D:190:TYR:HD1	2.26	0.43
1:A:142:ASP:OD1	1:A:142:ASP:C	2.62	0.42
1:D:11:ILE:HG12	1:D:183:VAL:HG12	2.01	0.42
1:D:120:LEU:HD13	1:D:151:PHE:CE2	2.55	0.42
1:A:56:MET:HE1	1:B:63:ARG:HG3	2.00	0.42
1:B:198:GLN:HA	1:B:201:GLN:NE2	2.34	0.42
1:D:15:GLU:OE1	1:D:180:ARG:HB3	2.19	0.42
1:B:79:VAL:HG12	1:B:91:GLN:HB3	2.01	0.42
1:B:116:THR:O	1:B:117:ALA:HB3	2.18	0.42
1:B:121:ASN:ND2	1:B:149:VAL:HG21	2.33	0.42
1:B:197:ARG:C	1:B:199:LYS:H	2.28	0.42
1:C:142:ASP:OD1	1:C:142:ASP:C	2.62	0.42
1:A:51:LEU:HA	1:A:52:ARG:HA	1.72	0.42
1:C:67:ASP:C	1:C:69:ASN:H	2.28	0.42
1:D:10:LYS:HE2	1:D:12:LEU:HD23	2.01	0.42
1:D:177:ARG:NH1	1:D:177:ARG:HG2	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:VAL:HG22	1:B:77:ILE:HD11	2.00	0.42
1:B:121:ASN:HD22	1:B:149:VAL:HG21	1.85	0.42
1:A:27:LYS:CD	1:A:68:PHE:CE2	3.03	0.42
1:B:131:ARG:NH2	1:D:118:LEU:HD22	2.35	0.42
1:A:27:LYS:HE3	3:A:3010:HOH:O	2.19	0.42
1:D:114:VAL:HG12	1:D:139:VAL:HG21	2.02	0.42
1:D:137:THR:HG22	1:D:153:ALA:HB1	2.02	0.42
1:A:28:ARG:NH1	1:A:28:ARG:CG	2.61	0.41
1:B:128:PHE:HB2	1:B:135:LEU:HD23	2.02	0.41
1:C:14:THR:O	1:C:15:GLU:C	2.62	0.41
1:A:87:THR:HG23	1:A:89:SER:HB3	2.01	0.41
1:C:194:GLU:OE1	1:C:194:GLU:HA	2.20	0.41
1:D:114:VAL:O	1:D:114:VAL:HG13	2.18	0.41
1:D:162:ASN:N	1:D:162:ASN:ND2	2.69	0.41
1:A:7:PHE:O	1:A:186:ARG:HG2	2.20	0.41
1:A:116:THR:O	1:A:117:ALA:HB3	2.19	0.41
1:B:82:TYR:CE2	1:B:93:ARG:HB2	2.56	0.41
1:C:82:TYR:CE1	1:C:93:ARG:HG3	2.56	0.41
1:D:14:THR:O	1:D:18:ILE:HG13	2.20	0.41
1:B:137:THR:HG22	1:B:153:ALA:HB1	2.02	0.41
1:B:52:ARG:H	1:B:52:ARG:HG2	1.62	0.41
1:A:41:TYR:CB	1:B:193:ARG:HH21	2.29	0.41
1:B:28:ARG:HD3	3:B:3111:HOH:O	2.19	0.41
1:B:120:LEU:HD13	1:B:151:PHE:HE2	1.86	0.41
1:B:136:LYS:HG3	1:B:154:ASP:OD1	2.21	0.41
1:B:144:ARG:CD	1:B:159:ASN:HD22	2.29	0.41
1:C:77:ILE:O	1:C:77:ILE:HG13	2.20	0.41
1:B:115:ASP:OD1	1:B:115:ASP:C	2.64	0.41
1:D:113:ILE:HG23	2:D:3003:IMP:H2'	2.02	0.41
1:A:197:ARG:O	1:A:197:ARG:CG	2.67	0.40
1:D:166:ILE:HD12	1:D:176:TYR:CG	2.56	0.40
1:A:80:SER:OG	1:B:99:ARG:NH1	2.55	0.40
1:C:56:MET:HE2	1:D:63:ARG:HG3	2.02	0.40
1:C:148:ARG:HD2	1:C:148:ARG:HA	1.90	0.40
1:C:27:LYS:HD3	1:C:68:PHE:CE2	2.56	0.40
1:A:175:THR:CG2	1:A:176:TYR:N	2.83	0.40
1:C:11:ILE:N	1:C:11:ILE:CD1	2.85	0.40
1:C:140:LEU:HD21	1:C:168:TYR:CD2	2.53	0.40
1:D:121:ASN:ND2	1:D:149:VAL:HG21	2.37	0.40
1:B:92:VAL:HG11	1:D:130:ARG:CG	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ARG:NH1	1:B:186:ARG:NH1[2_555]	2.00	0.20

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	190/221 (86%)	176 (93%)	13 (7%)	1 (0%)	24	48
1	B	200/221 (90%)	183 (92%)	13 (6%)	4 (2%)	6	16
1	C	188/221 (85%)	174 (93%)	13 (7%)	1 (0%)	24	48
1	D	184/221 (83%)	168 (91%)	15 (8%)	1 (0%)	24	48
All	All	762/884 (86%)	701 (92%)	54 (7%)	7 (1%)	14	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	144	ARG
1	D	144	ARG
1	A	162	ASN
1	B	204	ILE
1	B	206	SER
1	C	162	ASN
1	B	202	ARG

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	169/194 (87%)	158 (94%)	11 (6%)	15	37
1	B	176/194 (91%)	166 (94%)	10 (6%)	18	43
1	C	167/194 (86%)	152 (91%)	15 (9%)	9	23
1	D	165/194 (85%)	155 (94%)	10 (6%)	17	40
All	All	677/776 (87%)	631 (93%)	46 (7%)	14	35

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	11	ILE
1	A	12	LEU
1	A	16	GLU
1	A	21	ARG
1	A	24	GLU
1	A	28	ARG
1	A	39	ARG
1	A	42	VAL
1	A	52	ARG
1	A	159	ASN
1	B	9	GLU
1	B	43	ASN
1	B	52	ARG
1	B	99	ARG
1	B	136	LYS
1	B	137	THR
1	B	152	SER
1	B	192	GLU
1	B	193	ARG
1	B	201	GLN
1	C	10	LYS
1	C	11	ILE
1	C	12	LEU
1	C	16	GLU
1	C	21	ARG
1	C	24	GLU
1	C	28	ARG
1	C	38	LEU
1	C	39	ARG
1	C	42	VAL
1	C	52	ARG
1	C	93	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	138	VAL
1	C	159	ASN
1	C	193	ARG
1	D	9	GLU
1	D	43	ASN
1	D	52	ARG
1	D	99	ARG
1	D	130	ARG
1	D	136	LYS
1	D	137	THR
1	D	152	SER
1	D	177	ARG
1	D	192	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	159	ASN
1	A	162	ASN
1	B	43	ASN
1	B	91	GLN
1	B	100	HIS
1	B	121	ASN
1	B	159	ASN
1	B	162	ASN
1	B	198	GLN
1	B	201	GLN
1	C	91	GLN
1	C	159	ASN
1	C	162	ASN
1	D	43	ASN
1	D	125	HIS
1	D	159	ASN
1	D	162	ASN
1	D	198	GLN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	IMP	C	3002	-	25,25,25	0.58	0	37,38,38	0.55	0
2	IMP	B	3001	-	25,25,25	0.56	0	37,38,38	0.61	0
2	IMP	A	3000	-	25,25,25	0.58	0	37,38,38	0.55	0
2	IMP	D	3003	-	25,25,25	0.65	0	37,38,38	0.59	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	IMP	C	3002	-	-	3/10/26/26	0/3/3/3
2	IMP	B	3001	-	-	3/10/26/26	0/3/3/3
2	IMP	A	3000	-	-	0/10/26/26	0/3/3/3
2	IMP	D	3003	-	-	3/10/26/26	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3001	IMP	C5'-O5'-P-O1P
2	B	3001	IMP	C5'-O5'-P-O2P
2	B	3001	IMP	C5'-O5'-P-O3P
2	C	3002	IMP	C5'-O5'-P-O1P
2	C	3002	IMP	C5'-O5'-P-O2P
2	C	3002	IMP	C5'-O5'-P-O3P
2	D	3003	IMP	C5'-O5'-P-O1P
2	D	3003	IMP	C5'-O5'-P-O2P
2	D	3003	IMP	C5'-O5'-P-O3P

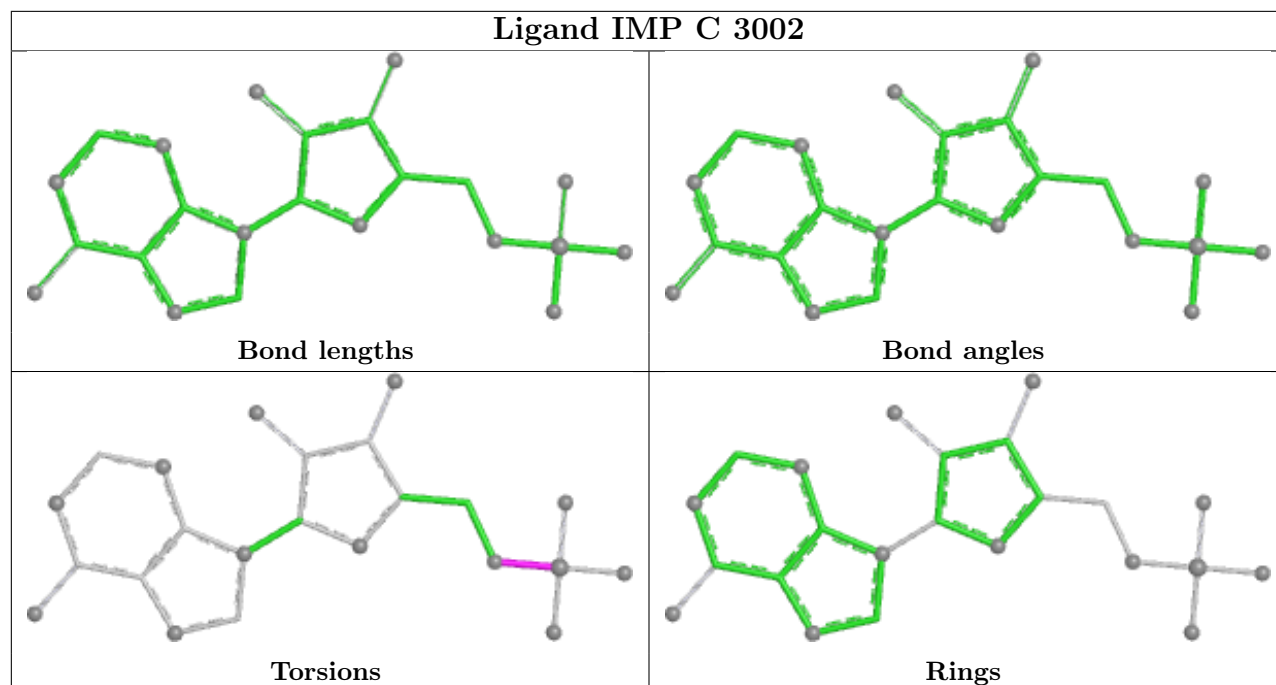
There are no ring outliers.

3 monomers are involved in 3 short contacts:

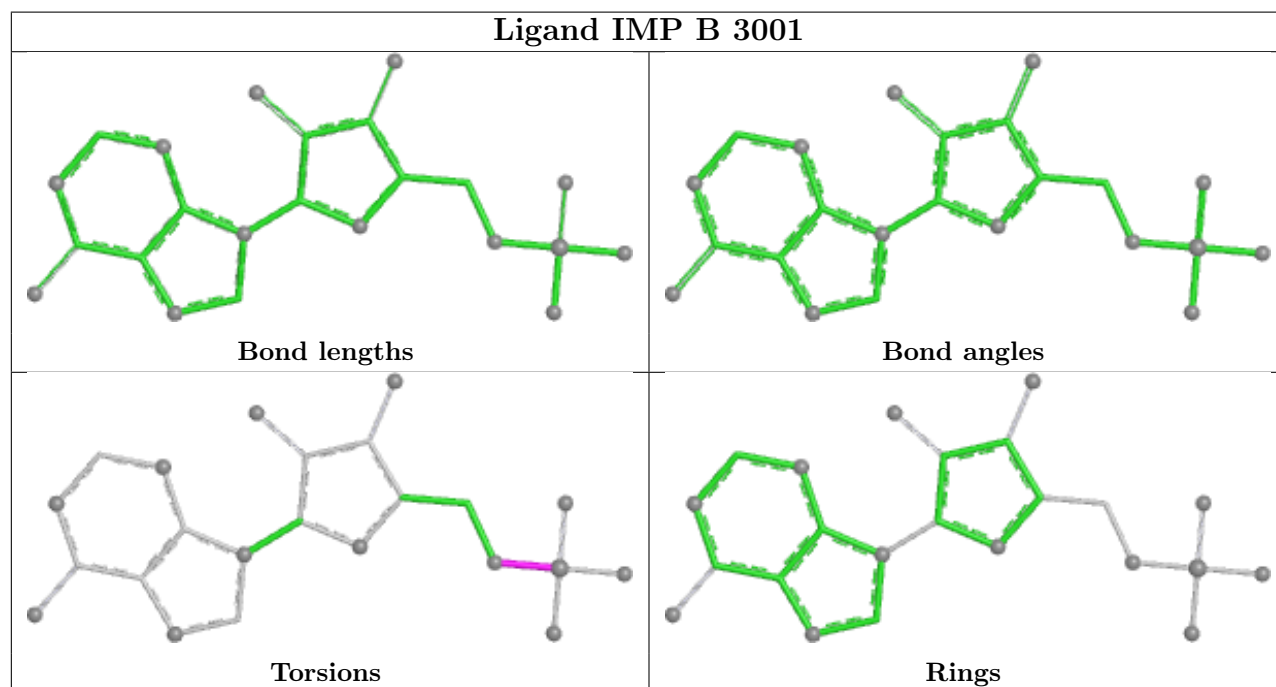
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3002	IMP	1	0
2	A	3000	IMP	1	0
2	D	3003	IMP	1	0

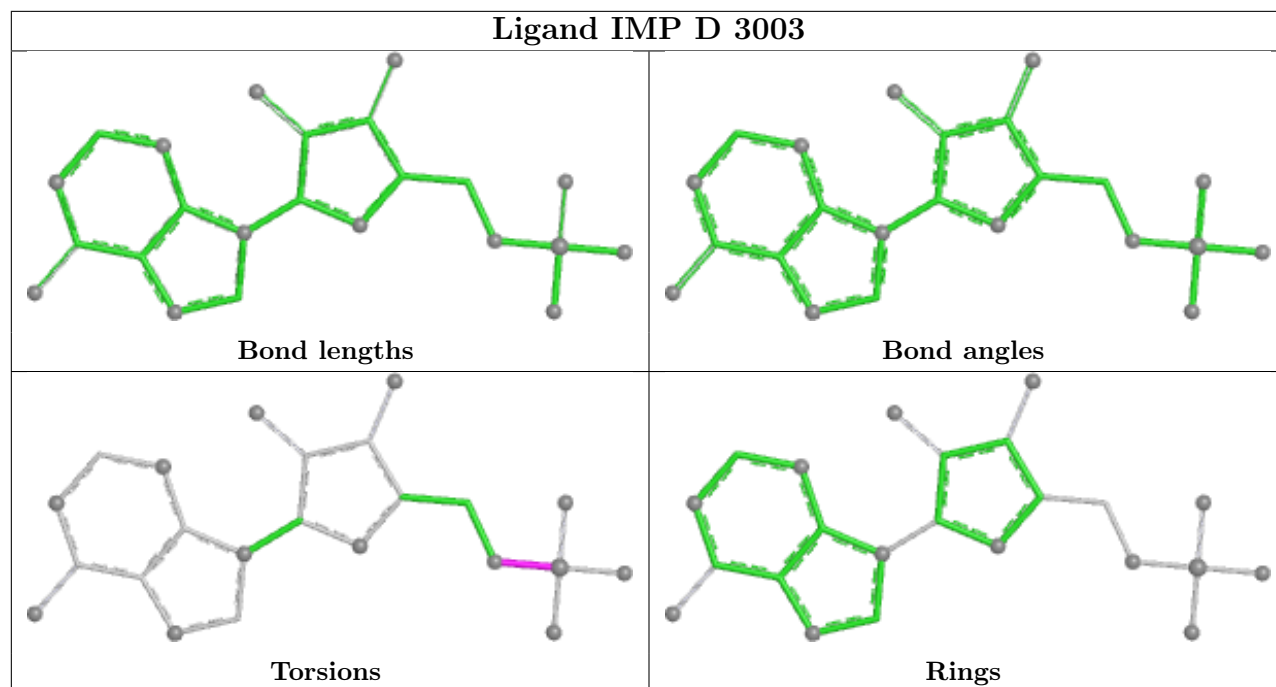
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 IMP C 3002



Ligand IMP B 3001





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.