Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2023 – 10:51 PM EDT

PDB ID	:	1JFS
Title	:	PURINE REPRESSOR MUTANT-HYPOXANTHINE-PURF OPERATOR COMPLEX
Authors	:	Huffman, J.L.; Lu, F.; Zalkin, H.; Brennan, R.G.
Deposited on	:	2001-06-21
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:

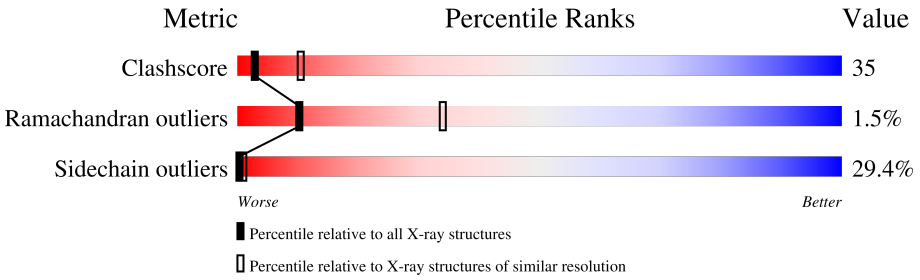
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	17	41% 59%
2	A	340	35% 47% 17% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3040 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 DNA chain called 5'-D(*TP*AP*CP*GP*CP*AP*AP*AP*CP*GP*TP*TP*TP*GP*CP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	17	345	166	62	101	16	0	0	0

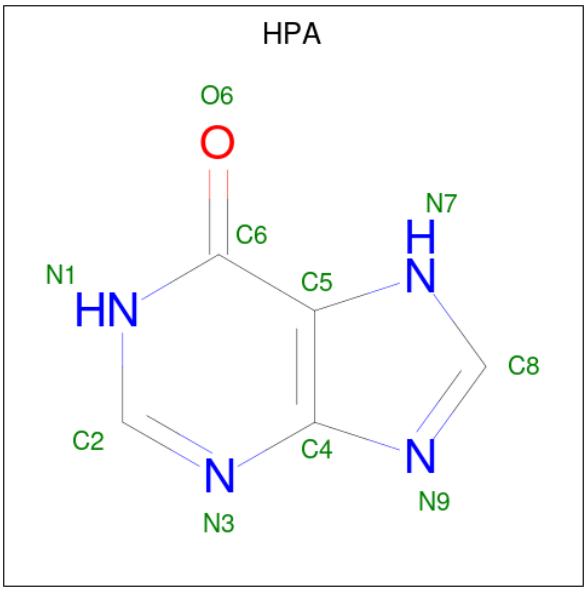
- Molecule 2 is a protein called PURINE NUCLEOTIDE SYNTHESIS REPRESSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	339	2654	1672	469	494	19	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	PHE	TRP	engineered mutation	UNP P0ACP7

- Molecule 3 is HYPOXANTHINE (three-letter code: HPA) (formula: $C_5H_4N_4O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 10 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	3	Total O 3 3	0	0
4	A	28	Total O 28 28	0	0

3 Residue-property plots (i)

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

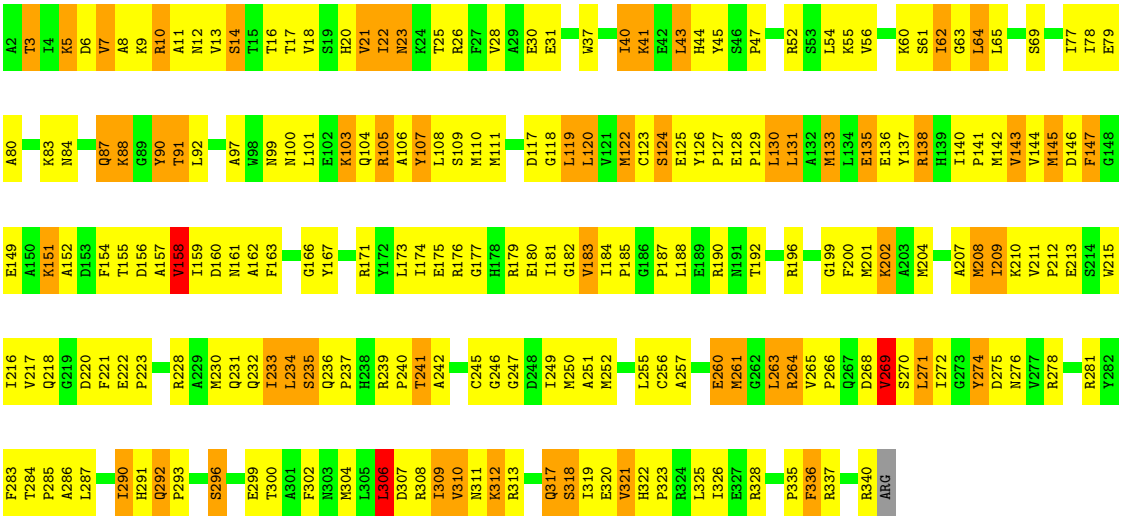
Note EDS was not executed.

• Molecule 1: 5'-D(*TP*AP*CP*GP*CP*AP*AP*AP*CP*GP*TP*TP*TP*GP*CP*GP*T)-3
'

Chain B:

• Molecule 2: PURINE NUCLEOTIDE SYNTHESIS REPRESSOR

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	176.05Å 95.04Å 81.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	97.9 (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	7.54	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.157 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3040	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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: HPA

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	B	1.82	9/386 (2.3%)	4.11	81/594 (13.6%)
2	A	0.91	0/2707	1.01	5/3660 (0.1%)
All	All	1.06	9/3093 (0.3%)	1.80	86/4254 (2.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	706	DA	N3-C4	-7.24	1.30	1.34
1	B	705	DA	C3'-O3'	-6.58	1.35	1.44
1	B	702	DG	C3'-O3'	6.27	1.52	1.44
1	B	701	DC	C1'-N1	-5.98	1.38	1.47
1	B	701	DC	C4-C5	5.53	1.47	1.43
1	B	699	DT	N1-C2	5.46	1.42	1.38
1	B	706	DA	C6-N1	-5.35	1.31	1.35
1	B	702	DG	C5-C6	-5.29	1.37	1.42
1	B	712	DG	C3'-O3'	5.09	1.50	1.44

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	715	DT	C6-N1-C1'	-22.95	85.97	120.40
1	B	700	DA	C8-N9-C1'	-19.94	91.81	127.70
1	B	714	DG	C4-N9-C1'	-19.46	101.20	126.50
1	B	715	DT	C2-N1-C1'	19.23	148.96	118.20
1	B	714	DG	C8-N9-C1'	18.41	150.93	127.00
1	B	700	DA	C4-N9-C1'	18.06	158.80	126.30
1	B	712	DG	C4-N9-C1'	-16.16	105.48	126.50
1	B	712	DG	C8-N9-C1'	16.11	147.95	127.00
1	B	701	DC	C6-N1-C1'	-15.44	102.27	120.80
1	B	701	DC	C2-N1-C1'	13.88	134.06	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	706	DA	C8-N9-C1'	13.86	152.64	127.70
1	B	706	DA	C4-N9-C1'	-13.27	102.42	126.30
1	B	702	DG	C4-N9-C1'	12.61	142.90	126.50
1	B	700	DA	C1'-O4'-C4'	-12.60	97.50	110.10
1	B	702	DG	C8-N9-C1'	-12.51	110.74	127.00
1	B	702	DG	O4'-C1'-C2'	-11.22	96.92	105.90
1	B	711	DT	C2-N1-C1'	-10.87	100.80	118.20
1	B	707	DC	C2-N1-C1'	-10.77	106.96	118.80
1	B	711	DT	C6-N1-C1'	10.55	136.22	120.40
1	B	715	DT	O4'-C1'-N1	10.35	115.24	108.00
1	B	707	DC	C6-N1-C1'	10.11	132.93	120.80
1	B	700	DA	O4'-C4'-C3'	-9.97	100.02	106.00
1	B	702	DG	C5-C6-O6	-9.94	122.64	128.60
1	B	704	DA	C4-N9-C1'	-9.88	108.52	126.30
1	B	713	DC	C2-N1-C1'	-9.84	107.98	118.80
1	B	702	DG	C4-C5-N7	9.78	114.71	110.80
1	B	706	DA	P-O3'-C3'	9.76	131.41	119.70
1	B	701	DC	C1'-O4'-C4'	-9.56	100.54	110.10
1	B	705	DA	C4-N9-C1'	-9.21	109.72	126.30
1	B	713	DC	P-O5'-C5'	-9.14	106.27	120.90
1	B	704	DA	C8-N9-C1'	9.01	143.91	127.70
1	B	703	DC	C4'-C3'-C2'	-8.98	95.02	103.10
1	B	705	DA	C8-N9-C1'	8.90	143.73	127.70
1	B	699	DT	N3-C2-O2	-8.79	117.03	122.30
1	B	700	DA	C8-N9-C4	8.63	109.25	105.80
1	B	702	DG	C4'-C3'-C2'	-8.37	95.57	103.10
1	B	712	DG	P-O3'-C3'	8.04	129.35	119.70
1	B	701	DC	C6-N1-C2	8.03	123.51	120.30
1	B	703	DC	P-O3'-C3'	7.91	129.19	119.70
2	A	269	VAL	CB-CA-C	-7.87	96.45	111.40
1	B	712	DG	C2-N3-C4	-7.68	108.06	111.90
1	B	713	DC	C6-N1-C2	7.61	123.34	120.30
2	A	340	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	699	DT	C5-C6-N1	-7.32	119.31	123.70
1	B	700	DA	N7-C8-N9	-7.11	110.25	113.80
1	B	702	DG	C6-C5-N7	-7.04	126.18	130.40
1	B	712	DG	C5-C6-N1	-6.91	108.04	111.50
1	B	710	DT	P-O5'-C5'	-6.83	109.97	120.90
1	B	709	DT	C6-N1-C1'	-6.77	110.25	120.40
1	B	699	DT	C2-N3-C4	-6.60	123.24	127.20
1	B	699	DT	C6-C5-C7	-6.52	118.99	122.90
1	B	702	DG	C5-N7-C8	-6.49	101.05	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	711	DT	C6-C5-C7	-6.43	119.04	122.90
1	B	699	DT	C4-C5-C6	6.36	121.81	118.00
1	B	702	DG	P-O3'-C3'	6.33	127.30	119.70
1	B	712	DG	O4'-C1'-N9	-5.99	103.81	108.00
1	B	704	DA	P-O5'-C5'	-5.99	111.32	120.90
1	B	714	DG	C4'-C3'-C2'	5.98	108.48	103.10
1	B	705	DA	C2-N3-C4	-5.94	107.63	110.60
1	B	701	DC	P-O5'-C5'	5.82	130.21	120.90
1	B	708	DG	O4'-C1'-C2'	5.80	110.54	105.90
1	B	699	DT	O3'-P-O5'	-5.77	93.04	104.00
1	B	715	DT	C1'-O4'-C4'	-5.76	104.34	110.10
1	B	703	DC	C2-N1-C1'	5.73	125.10	118.80
1	B	700	DA	O3'-P-O5'	-5.72	93.13	104.00
2	A	290	ILE	CB-CA-C	-5.68	100.24	111.60
1	B	699	DT	N1-C2-N3	5.68	118.01	114.60
1	B	699	DT	N3-C4-O4	-5.65	116.51	119.90
1	B	713	DC	C5-C6-N1	-5.60	118.20	121.00
2	A	158	VAL	N-CA-C	-5.48	96.20	111.00
1	B	701	DC	C2-N3-C4	-5.46	117.17	119.90
1	B	701	DC	N3-C4-C5	5.44	124.08	121.90
1	B	710	DT	C3'-C2'-C1'	-5.33	96.11	102.50
1	B	713	DC	C6-N1-C1'	5.33	127.19	120.80
2	A	306	LEU	CA-CB-CG	-5.33	103.05	115.30
1	B	708	DG	C5-C6-O6	-5.32	125.41	128.60
1	B	702	DG	C5-C6-N1	5.30	114.15	111.50
1	B	702	DG	N1-C6-O6	5.29	123.08	119.90
1	B	709	DT	C2-N1-C1'	5.29	126.66	118.20
1	B	708	DG	O3'-P-O5'	-5.26	94.01	104.00
1	B	707	DC	O4'-C1'-N1	-5.26	104.32	108.00
1	B	708	DG	C8-N9-C1'	-5.21	120.23	127.00
1	B	701	DC	C5-C6-N1	-5.18	118.41	121.00
1	B	705	DA	P-O5'-C5'	-5.09	112.76	120.90
1	B	708	DG	C5-C6-N1	5.07	114.03	111.50
1	B	703	DC	O4'-C1'-C2'	-5.01	101.89	105.90

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	B	345	0	194	14	0
2	A	2654	0	2640	193	0
3	A	10	0	4	0	0
4	A	28	0	0	1	0
4	B	3	0	0	0	0
All	All	3040	0	2838	206	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 35.

All (206) 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:713:DC:H2"	1:B:714:DG:H5"	1.41	0.99
2:A:236:GLN:HB2	2:A:237:PRO:HD2	1.50	0.94
1:B:712:DG:H2"	1:B:713:DC:H5"	1.52	0.90
2:A:100:ASN:HD22	2:A:103:LYS:H	1.13	0.89
2:A:20:HIS:ND1	2:A:25:THR:HG23	1.87	0.88
2:A:142:MET:HG3	2:A:155:THR:HG22	1.58	0.83
2:A:22:ILE:HG22	2:A:23:ASN:ND2	1.92	0.83
2:A:292:GLN:HG3	2:A:293:PRO:HD2	1.60	0.83
2:A:97:ALA:HB1	2:A:104:GLN:HG3	1.62	0.82
2:A:192:THR:O	2:A:196:ARG:HD2	1.81	0.81
2:A:10:ARG:HG3	2:A:10:ARG:HH11	1.47	0.80
2:A:135:GLU:O	2:A:138:ARG:HG2	1.84	0.77
2:A:107:TYR:O	2:A:111:MET:HG3	1.84	0.76
2:A:137:TYR:HB3	2:A:140:ILE:CD1	2.15	0.76
2:A:100:ASN:ND2	2:A:103:LYS:H	1.83	0.76
2:A:143:VAL:HB	2:A:156:ASP:HB2	1.68	0.75
2:A:247:GLY:HA2	2:A:274:TYR:O	1.88	0.74
2:A:234:LEU:HD22	2:A:263:LEU:HD23	1.70	0.74
2:A:196:ARG:HG2	2:A:274:TYR:CE1	2.24	0.73
2:A:160:ASP:HA	2:A:321:VAL:HG23	1.71	0.72
2:A:145:MET:HA	2:A:158:VAL:CG1	2.20	0.72
2:A:62:ILE:HD12	2:A:90:TYR:CD1	2.25	0.71
2:A:159:ILE:HG13	2:A:320:GLU:HA	1.71	0.71
2:A:97:ALA:CB	2:A:104:GLN:HG3	2.21	0.69
2:A:61:SER:HB2	2:A:91:THR:HG22	1.74	0.69
1:B:714:DG:H4'	1:B:714:DG:OP1	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:LEU:O	2:A:328:ARG:HD2	1.92	0.69
2:A:137:TYR:HB3	2:A:140:ILE:HD13	1.74	0.69
2:A:236:GLN:HB2	2:A:237:PRO:CD	2.23	0.68
2:A:20:HIS:HA	2:A:25:THR:CG2	2.23	0.67
2:A:40:ILE:HD13	2:A:45:TYR:HD1	1.57	0.67
2:A:266:PRO:HA	2:A:269:VAL:O	1.94	0.67
2:A:207:ALA:HB3	2:A:209:ILE:HG13	1.77	0.66
2:A:21:VAL:HG12	2:A:28:VAL:HG21	1.76	0.66
1:B:712:DG:H2"	1:B:713:DC:C5'	2.26	0.66
2:A:61:SER:CB	2:A:91:THR:HG22	2.25	0.66
2:A:156:ASP:HB3	2:A:304:MET:CE	2.26	0.65
2:A:257:ALA:O	2:A:261:MET:HG3	1.96	0.65
2:A:292:GLN:HG3	2:A:293:PRO:CD	2.26	0.65
2:A:174:ILE:HG22	2:A:175:GLU:N	2.11	0.64
2:A:20:HIS:HA	2:A:25:THR:HG22	1.79	0.64
2:A:290:ILE:HD13	2:A:325:LEU:HD23	1.80	0.64
2:A:135:GLU:HA	2:A:154:PHE:CE1	2.32	0.64
1:B:709:DT:H2"	1:B:710:DT:H5'	1.78	0.64
2:A:87:GLN:OE1	2:A:88:LYS:HD2	1.99	0.62
2:A:200:PHE:HD2	2:A:201:MET:HE2	1.63	0.62
2:A:304:MET:CE	2:A:317:GLN:HB3	2.29	0.62
2:A:264:ARG:HB2	2:A:268:ASP:OD2	1.99	0.61
1:B:700:DA:H2"	1:B:701:DC:O5'	2.00	0.61
2:A:52:ARG:NH1	2:A:56:VAL:HG11	2.15	0.61
2:A:221:PHE:HA	2:A:250:MET:HG3	1.83	0.61
2:A:256:CYS:O	2:A:260:GLU:HG2	2.01	0.61
2:A:252:MET:HB2	2:A:283:PHE:CE2	2.35	0.61
2:A:152:ALA:HB1	2:A:154:PHE:CE2	2.36	0.60
2:A:101:LEU:HA	2:A:104:GLN:NE2	2.16	0.60
2:A:184:ILE:HA	2:A:217:VAL:O	2.01	0.60
2:A:156:ASP:HB3	2:A:304:MET:HE1	1.83	0.59
2:A:230:MET:O	2:A:234:LEU:HD12	2.03	0.59
2:A:78:ILE:HG22	2:A:79:GLU:N	2.16	0.59
2:A:43:LEU:N	2:A:43:LEU:HD23	2.17	0.58
2:A:308:ARG:O	2:A:312:LYS:HA	2.04	0.58
2:A:159:ILE:HD11	2:A:320:GLU:CG	2.33	0.58
2:A:8:ALA:HB1	2:A:13:VAL:O	2.04	0.57
2:A:286:ALA:HB1	2:A:328:ARG:HD3	1.85	0.57
2:A:245:CYS:HB2	2:A:271:LEU:HD11	1.85	0.57
2:A:142:MET:CG	2:A:155:THR:HG22	2.33	0.57
2:A:325:LEU:HD22	2:A:326:ILE:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3:THR:HG23	2:A:5:LYS:H	1.70	0.56
2:A:166:GLY:HA3	2:A:196:ARG:O	2.06	0.56
2:A:167:TYR:CD2	2:A:202:LYS:HG3	2.41	0.56
2:A:37:TRP:HA	2:A:37:TRP:CE3	2.41	0.56
2:A:117:ASP:O	2:A:141:PRO:HG2	2.05	0.56
2:A:127:PRO:HB2	2:A:129:PRO:HD2	1.87	0.56
2:A:101:LEU:HA	2:A:104:GLN:HE21	1.70	0.56
2:A:304:MET:HE3	2:A:317:GLN:HB3	1.88	0.55
2:A:105:ARG:NH1	2:A:133:MET:HE2	2.22	0.55
2:A:3:THR:HG22	2:A:6:ASP:OD2	2.06	0.55
2:A:100:ASN:HB3	2:A:103:LYS:HB2	1.89	0.54
2:A:63:GLY:O	2:A:119:LEU:HD22	2.08	0.54
2:A:207:ALA:O	2:A:208:MET:HB2	2.07	0.54
2:A:304:MET:O	2:A:307:ASP:HB3	2.08	0.54
2:A:215:TRP:CE2	2:A:240:PRO:HD3	2.43	0.54
2:A:3:THR:HG22	2:A:6:ASP:H	1.73	0.53
2:A:10:ARG:HH11	2:A:10:ARG:CG	2.21	0.53
2:A:159:ILE:HD11	2:A:320:GLU:CD	2.28	0.53
2:A:7:VAL:HG12	2:A:18:VAL:HG21	1.91	0.53
2:A:40:ILE:HD13	2:A:45:TYR:CD1	2.42	0.53
2:A:336:PHE:N	2:A:336:PHE:CD1	2.77	0.53
2:A:163:PHE:O	2:A:199:GLY:HA3	2.09	0.52
2:A:23:ASN:N	2:A:23:ASN:HD22	2.08	0.52
2:A:239:ARG:HB2	2:A:240:PRO:HD2	1.91	0.52
2:A:304:MET:SD	2:A:319:ILE:HD12	2.49	0.52
2:A:187:PRO:HD3	2:A:220:ASP:HA	1.91	0.52
2:A:90:TYR:N	2:A:90:TYR:CD2	2.78	0.52
2:A:245:CYS:SG	2:A:251:ALA:HA	2.51	0.51
2:A:158:VAL:HG13	2:A:158:VAL:O	2.11	0.51
2:A:16:THR:HG22	2:A:20:HIS:HD2	1.76	0.51
2:A:11:ALA:HB3	2:A:13:VAL:HG22	1.93	0.51
2:A:101:LEU:HD11	2:A:133:MET:HE3	1.92	0.51
2:A:122:MET:HA	2:A:146:ASP:OD1	2.10	0.51
2:A:222:GLU:HB3	2:A:223:PRO:HD2	1.93	0.51
2:A:231:GLN:O	2:A:235:SER:HB2	2.11	0.50
2:A:308:ARG:HA	2:A:313:ARG:HB3	1.92	0.50
1:B:711:DT:H2"	1:B:712:DG:N7	2.26	0.50
2:A:11:ALA:O	2:A:12:ASN:HB2	2.10	0.50
2:A:62:ILE:HD12	2:A:90:TYR:HD1	1.72	0.50
2:A:220:ASP:O	2:A:221:PHE:HB2	2.11	0.50
2:A:41:LYS:N	2:A:41:LYS:HD2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:187:PRO:HA	2:A:218:GLN:NE2	2.27	0.50
2:A:296:SER:O	2:A:300:THR:HB	2.12	0.50
2:A:126:TYR:CG	2:A:147:PHE:HE2	2.30	0.49
2:A:158:VAL:HA	2:A:319:ILE:O	2.12	0.49
2:A:179:ARG:HA	2:A:209:ILE:CD1	2.41	0.49
1:B:702:DG:O5'	1:B:702:DG:H2'	2.11	0.49
2:A:180:GLU:HB2	2:A:241:THR:HG23	1.93	0.49
2:A:135:GLU:HA	2:A:154:PHE:CZ	2.48	0.49
2:A:160:ASP:O	2:A:161:ASN:HB2	2.12	0.49
2:A:10:ARG:HG3	2:A:10:ARG:NH1	2.21	0.49
2:A:118:GLY:HA2	2:A:141:PRO:HD2	1.93	0.49
2:A:100:ASN:HD22	2:A:103:LYS:N	1.95	0.49
2:A:233:ILE:HG22	2:A:234:LEU:HG	1.95	0.49
2:A:65:LEU:HD22	2:A:108:LEU:HD13	1.95	0.48
2:A:159:ILE:HG13	2:A:159:ILE:O	2.13	0.48
1:B:709:DT:H2"	1:B:710:DT:C5'	2.44	0.48
1:B:714:DG:C2'	1:B:715:DT:H5'	2.43	0.48
2:A:16:THR:HG22	2:A:20:HIS:CD2	2.49	0.48
2:A:185:PRO:HD2	2:A:218:GLN:HA	1.96	0.48
2:A:179:ARG:HA	2:A:209:ILE:HD13	1.96	0.47
2:A:123:CYS:HB2	2:A:126:TYR:CE2	2.48	0.47
2:A:200:PHE:CZ	2:A:204:MET:HE3	2.50	0.47
2:A:147:PHE:CD1	2:A:151:LYS:HB2	2.50	0.47
2:A:135:GLU:OE2	2:A:138:ARG:HD2	2.14	0.46
2:A:77:ILE:HG21	2:A:122:MET:CE	2.45	0.46
2:A:140:ILE:HD12	2:A:140:ILE:H	1.79	0.46
2:A:187:PRO:HD2	2:A:221:PHE:CE2	2.50	0.46
1:B:702:DG:OP2	2:A:14:SER:HB3	2.16	0.46
2:A:171:ARG:O	2:A:174:ILE:HB	2.16	0.46
2:A:167:TYR:HD2	2:A:202:LYS:HG3	1.80	0.46
2:A:181:ILE:HG22	2:A:182:GLY:N	2.31	0.46
2:A:310:VAL:CG2	2:A:311:ASN:N	2.78	0.46
1:B:714:DG:H2"	1:B:715:DT:H5'	1.98	0.45
2:A:126:TYR:CD1	2:A:147:PHE:HE2	2.35	0.45
2:A:271:LEU:HD12	2:A:272:ILE:N	2.30	0.45
2:A:325:LEU:HD22	2:A:326:ILE:H	1.81	0.45
2:A:52:ARG:O	2:A:56:VAL:HG22	2.16	0.45
2:A:131:LEU:HD12	2:A:131:LEU:HA	1.72	0.45
2:A:322:HIS:HA	2:A:323:PRO:HD3	1.71	0.45
2:A:157:ALA:O	2:A:318:SER:HA	2.17	0.45
2:A:335:PRO:HB2	2:A:336:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:173:LEU:HD13	2:A:181:ILE:HD13	1.98	0.45
2:A:335:PRO:HB2	2:A:336:PHE:CE1	2.52	0.45
1:B:710:DT:H2'	1:B:710:DT:O5'	2.16	0.44
2:A:100:ASN:HB3	2:A:103:LYS:CB	2.47	0.44
2:A:263:LEU:HD12	2:A:263:LEU:HA	1.57	0.44
2:A:17:THR:O	2:A:21:VAL:HG13	2.17	0.44
2:A:306:LEU:HA	2:A:306:LEU:HD12	1.10	0.44
2:A:310:VAL:HG23	2:A:311:ASN:OD1	2.18	0.44
2:A:41:LYS:HD2	2:A:41:LYS:HA	1.75	0.44
2:A:100:ASN:ND2	2:A:103:LYS:HB2	2.33	0.44
2:A:126:TYR:CD2	2:A:130:LEU:HD12	2.53	0.44
2:A:177:GLY:O	2:A:336:PHE:HD1	2.01	0.44
2:A:207:ALA:CB	2:A:209:ILE:HG13	2.45	0.44
2:A:120:LEU:HD12	2:A:120:LEU:HA	1.55	0.43
2:A:120:LEU:CD1	2:A:143:VAL:HG13	2.48	0.43
2:A:126:TYR:CD1	2:A:147:PHE:CE2	3.06	0.43
2:A:265:VAL:HA	2:A:266:PRO:HA	1.54	0.43
2:A:84:ASN:HB3	2:A:302:PHE:CD2	2.54	0.43
2:A:249:ILE:HG23	2:A:249:ILE:HD12	1.75	0.43
2:A:162:ALA:HB1	2:A:196:ARG:HG3	2.00	0.43
2:A:284:THR:HA	2:A:285:PRO:HA	1.81	0.43
2:A:43:LEU:HA	2:A:43:LEU:HD22	1.67	0.43
2:A:183:VAL:HG13	2:A:216:ILE:HG12	2.00	0.43
2:A:64:LEU:HD12	2:A:65:LEU:N	2.34	0.43
2:A:174:ILE:C	2:A:176:ARG:H	2.21	0.43
2:A:3:THR:HG22	2:A:6:ASP:CG	2.39	0.43
2:A:284:THR:O	2:A:284:THR:HG22	2.18	0.43
2:A:181:ILE:HA	2:A:242:ALA:O	2.19	0.42
2:A:187:PRO:HG2	2:A:190:ARG:HD3	2.01	0.42
2:A:188:LEU:HD23	2:A:188:LEU:HA	1.69	0.42
1:B:715:DT:H6	1:B:715:DT:H2'	0.83	0.42
2:A:200:PHE:HD2	2:A:201:MET:CE	2.28	0.42
2:A:201:MET:HE2	2:A:201:MET:CA	2.49	0.42
2:A:106:ALA:O	2:A:110:MET:HG3	2.20	0.42
2:A:233:ILE:O	2:A:236:GLN:HG2	2.19	0.42
2:A:249:ILE:HD13	2:A:249:ILE:HA	1.75	0.42
2:A:11:ALA:CB	2:A:13:VAL:HG22	2.49	0.42
2:A:123:CYS:O	2:A:124:SER:HB2	2.20	0.42
2:A:276:ASN:HD22	2:A:291:HIS:CD2	2.37	0.42
2:A:107:TYR:HA	2:A:110:MET:HG3	2.01	0.42
2:A:101:LEU:O	2:A:104:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:10:ARG:CG	2:A:10:ARG:NH1	2.79	0.41
2:A:90:TYR:N	2:A:90:TYR:HD2	2.19	0.41
2:A:125:GLU:HG2	2:A:190:ARG:HD2	2.00	0.41
2:A:144:VAL:HG21	2:A:147:PHE:CD2	2.55	0.41
2:A:264:ARG:HD2	2:A:264:ARG:HA	1.64	0.41
2:A:3:THR:HG23	2:A:5:LYS:N	2.33	0.41
2:A:211:VAL:HA	2:A:212:PRO:HD3	1.86	0.41
2:A:126:TYR:HD2	2:A:130:LEU:HD12	1.86	0.41
2:A:23:ASN:ND2	2:A:23:ASN:N	2.68	0.41
2:A:45:TYR:CE1	2:A:47:PRO:HG3	2.56	0.41
2:A:105:ARG:HB2	2:A:133:MET:SD	2.61	0.41
2:A:167:TYR:CE2	2:A:202:LYS:HG3	2.56	0.41
2:A:80:ALA:O	2:A:83:LYS:HB2	2.21	0.41
2:A:21:VAL:CG2	2:A:22:ILE:N	2.82	0.40
2:A:45:TYR:HA	4:A:810:HOH:O	2.22	0.40
2:A:61:SER:CB	2:A:91:THR:CG2	2.98	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
2	A	337/340 (99%)	297 (88%)	35 (10%)	5 (2%)	10 34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	275	ASP
2	A	309	ILE
2	A	312	LYS
2	A	124	SER
2	A	246	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	279/280 (100%)	197 (71%)	82 (29%)	0 1

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	THR
2	A	5	LYS
2	A	7	VAL
2	A	9	LYS
2	A	10	ARG
2	A	14	SER
2	A	21	VAL
2	A	22	ILE
2	A	23	ASN
2	A	26	ARG
2	A	30	GLU
2	A	31	GLU
2	A	40	ILE
2	A	41	LYS
2	A	43	LEU
2	A	44	HIS
2	A	54	LEU
2	A	55	LYS
2	A	60	LYS
2	A	62	ILE
2	A	64	LEU
2	A	69	SER
2	A	87	GLN
2	A	88	LYS
2	A	90	TYR
2	A	91	THR
2	A	92	LEU
2	A	99	ASN
2	A	103	LYS
2	A	105	ARG

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Mol	Chain	Res	Type
2	A	107	TYR
2	A	109	SER
2	A	119	LEU
2	A	120	LEU
2	A	122	MET
2	A	128	GLU
2	A	130	LEU
2	A	131	LEU
2	A	133	MET
2	A	135	GLU
2	A	136	GLU
2	A	138	ARG
2	A	143	VAL
2	A	145	MET
2	A	147	PHE
2	A	149	GLU
2	A	151	LYS
2	A	158	VAL
2	A	183	VAL
2	A	202	LYS
2	A	208	MET
2	A	209	ILE
2	A	210	LYS
2	A	213	GLU
2	A	228	ARG
2	A	232	GLN
2	A	233	ILE
2	A	234	LEU
2	A	235	SER
2	A	241	THR
2	A	255	LEU
2	A	260	GLU
2	A	261	MET
2	A	263	LEU
2	A	264	ARG
2	A	269	VAL
2	A	270	SER
2	A	271	LEU
2	A	274	TYR
2	A	278	ARG
2	A	281	ARG
2	A	292	GLN

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Mol	Chain	Res	Type
2	A	296	SER
2	A	299	GLU
2	A	306	LEU
2	A	309	ILE
2	A	310	VAL
2	A	317	GLN
2	A	318	SER
2	A	321	VAL
2	A	336	PHE
2	A	337	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	23	ASN
2	A	34	ASN
2	A	58	HIS
2	A	84	ASN
2	A	100	ASN
2	A	104	GLN
2	A	218	GLN
2	A	291	HIS
2	A	292	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	HPA	A	599	-	8,11,11	1.77	2 (25%)	5,15,15	2.59	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HPA	A	599	-	-	-	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	599	HPA	C6-N1	3.68	1.39	1.33
3	A	599	HPA	C2-N1	2.25	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	599	HPA	C2-N1-C6	4.91	124.11	115.88
3	A	599	HPA	N3-C2-N1	-2.54	124.70	128.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.