



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 07:53 AM 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 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) : 2.23.2

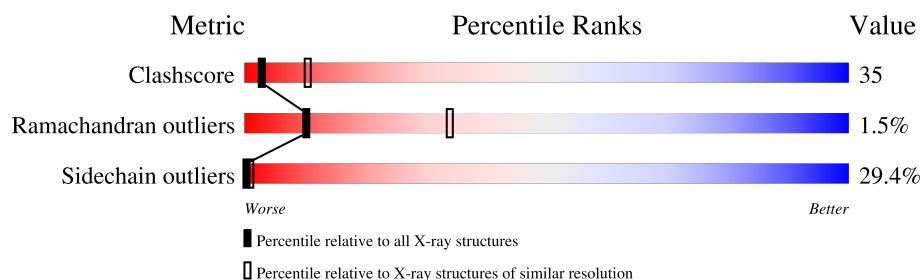
1 Overall quality at a glance

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))
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 $\leq 5\%$.

Note EDS was not executed.

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

2 Entry composition [i](#)

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
1	B	17	Total	C	N	O	P	0	0	0
			345	166	62	101	16			

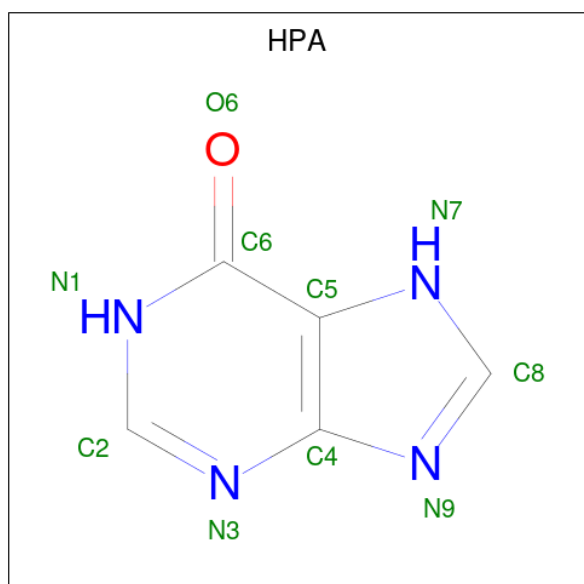
- Molecule 2 is a protein called PURINE NUCLEOTIDE SYNTHESIS REPRESSOR.

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

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: C₅H₄N₄O).



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

- Molecule 4 is water.

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

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: 5'-D(*TP*AP*CP*GP*CP*AP*AP*AP*CP*GP*TP*TP*TP*GP*CP*GP*T)-3',

Chain B: 

T699
A700
C701
G702
C703
A704
A705
A706
C707
G708
T709
T710
T711
G712
G713
G714
T715

- Molecule 2: PURINE NUCLEOTIDE SYNTHESIS REPRESSOR

Chain A: 

A2
T3
I4
K5
D6
V7
A8
K88
K9
R10
N11
N12
V13
S14
T15
T16
T17
V18
S19
H20
V21
I22
N23
K24
T25
R26
F27
V28
A29
E30
E31
W37
I40
K41
E42
L43
H44
Y45
S46
P47
R52
S53
L54
K55
V56
K60
S61
I62
G63
L64
L65
S69
I77
I78
E79

A80
K83
N84
Q87
K88
G89
Y90
T91
L92
A97
W96
N99
N100
T101
L101
E102
K103
Q104
R105
A106
Y107
L108
S109
M110
M111
D117
G118
L119
L120
V121
C122
C123
S124
E125
Y126
P127
E128
P129
L130
L131
A132
M133
L134
E135
E136
Y137
R138
H139
I140
P141
M142
V143
V144
M145
D146
F147
G148

E149
A150
K151
A152
D153
F154
T155
D156
A157
V158
I159
D160
N161
A162
F163
G166
Y167
R171
Y172
L173
I174
E175
R176
G177
H178
R179
E180
I181
G182
V183
I184
P185
G186
P187
L188
E189
R190
N191
T192
R196
G199
P200
M201
K202
A203
M204
A207
M208
I209
K210
V211
P212
E213
W215

I216
V217
G218
Q219
D220
F221
E222
P223
R228
A229
M230
Q231
Q232
L233
A234
Q235
Q236
P237
H238
R239
P240
T241
A242
C245
G246
G247
D248
I249
M250
A251
M252
L255
H256
C256
P323
R324
L325
I326
E327
R328
E260
M261
G262
L263
R264
V265
P266
Q267
D268
V269
S270
L271
I272
G273
Y274
D275
N276
V277
R278
R281
Y282

F283
T284
P285
A286
L287
I290
H291
Q292
P293
S296
E299
T300
A301
F302
R303
K304
L305
L306
D307
R308
I309
V310
N311
K312
R313
Q317
S318
I319
E320
V321
P322
P323
L325
I326
E327
R328
P335
F336
R337
R340
ARG

4 Data and refinement statistics

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(°)	Ideal(°)
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(°)	Ideal(°)
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(°)	Ideal(°)
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

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

5.3.1 Protein backbone

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 ⓘ

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(°)	Ideal(°)
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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.