Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 – 08:42 am BST

PDB ID	:	2ON3
Title	:	A structural insight into the inhibition of human and Leishmania donovani ornithine decarboxylases by 3-aminooxy-1-aminopropane
Authors	:	Dufe, V.T.; Ingner, D.; Heby, O.; Khomutov, A.R.; Persson, L.; Al-Karadaghi, S.
Deposited on	:	2007-01-23
Resolution	:	3.00 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

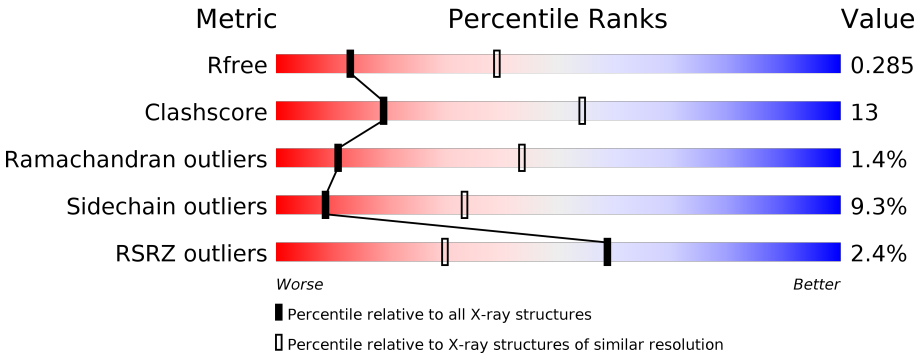
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	461	2% 59% 23% • 15%
1	B	461	2% 62% 20% • 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	XAP	A	601	-	-	X	-
2	XAP	B	601	-	-	X	-

2 Entry composition

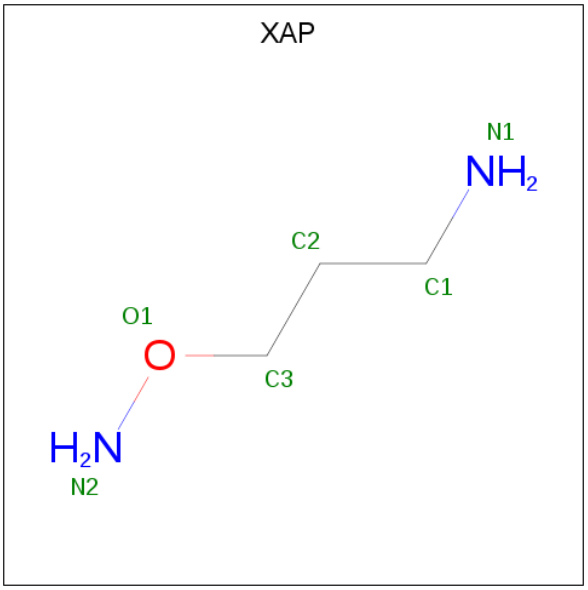
There are 2 unique types of molecules in this entry. The entry contains 6158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ornithine decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3073	1973	507	573	20			
1	B	392	Total	C	N	O	S	0	0	0
			3073	1973	507	573	20			

- Molecule 2 is 3-AMINOOXY-1-AMINOPROPANE (three-letter code: XAP) (formula: $C_3H_{10}N_2O$).



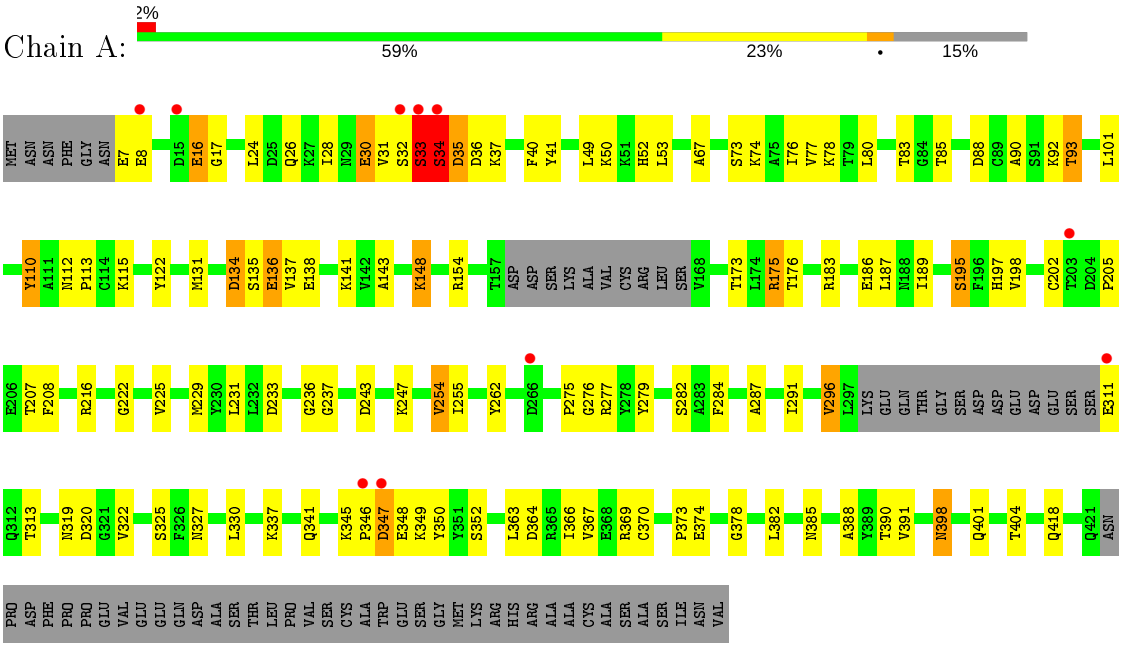
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			6	3	2	1		
2	B	1	Total	C	N	O	0	0
			6	3	2	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

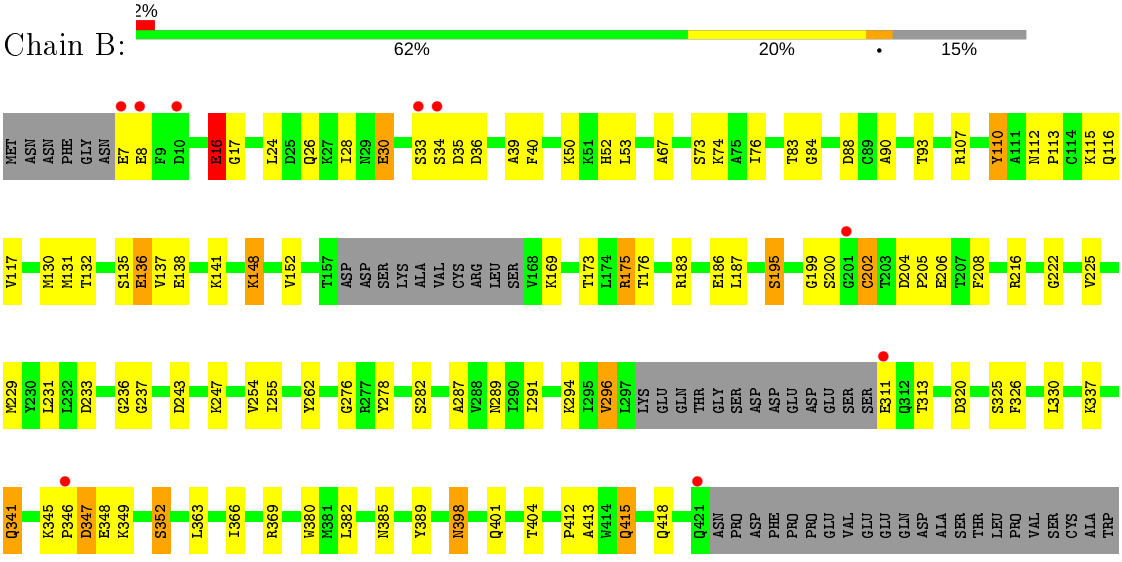
- Molecule 1: Ornithine decarboxylase

Chain A:



- Molecule 1: Ornithine decarboxylase

Chain B:



GLU
SER
GLY
MET
LYS
ARG
HIS
ARG
ALA
ALA
CYS
ALA
SER
ALA
SER
ILE
ASN
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.54Å 104.84Å 137.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.82 – 3.00 19.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.82-3.00) 100.0 (19.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.26 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.293 0.223 , 0.285	Depositor DCC
R_{free} test set	1806 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 30.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6158	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.68	0/3142	0.75	0/4253
1	B	0.70	0/3142	0.74	0/4253
All	All	0.69	0/6284	0.74	0/8506

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	35	ASP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	SER	Peptide

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	3073	0	3043	92	0
1	B	3073	0	3043	82	0
2	A	6	0	10	12	0
2	B	6	0	10	10	0
All	All	6158	0	6106	159	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 13.

All (159) 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:237:GLY:H	2:B:601:XAP:C1	1.75	0.99
1:B:237:GLY:H	2:B:601:XAP:H12	1.29	0.97
1:B:276:GLY:H	2:B:601:XAP:HN11	1.04	0.96
1:A:401:GLN:HE21	1:B:93:THR:HG21	1.32	0.93
1:A:277:ARG:H	2:A:601:XAP:H11	1.33	0.92
1:A:277:ARG:N	2:A:601:XAP:H11	1.88	0.87
1:A:26:GLN:O	1:A:30:GLU:HG2	1.81	0.80
2:A:601:XAP:H12	2:A:601:XAP:N2	1.98	0.77
1:B:222:GLY:HA3	1:B:229:MET:CE	2.15	0.77
1:A:282:SER:HA	1:A:385:ASN:HD22	1.51	0.76
1:A:34:SER:O	1:A:35:ASP:HB3	1.86	0.75
1:B:195:SER:HB2	1:B:233:ASP:HB3	1.70	0.74
1:A:93:THR:HG21	1:B:401:GLN:HE21	1.52	0.73
1:B:237:GLY:N	2:B:601:XAP:H12	2.03	0.73
1:A:37:LYS:NZ	1:A:378:GLY:O	2.21	0.73
1:B:276:GLY:N	2:B:601:XAP:HN11	1.85	0.73
1:A:401:GLN:NE2	1:B:93:THR:HG21	2.04	0.72
1:A:276:GLY:H	2:A:601:XAP:H22	1.54	0.72
1:B:16:GLU:HG3	1:B:17:GLY:H	1.56	0.69
1:B:282:SER:HA	1:B:385:ASN:HD22	1.56	0.69
1:A:31:VAL:O	1:A:31:VAL:HG12	1.91	0.69
1:B:236:GLY:HA3	2:B:601:XAP:H21	1.74	0.69
1:A:277:ARG:HG2	2:A:601:XAP:H12	1.76	0.67
1:B:26:GLN:O	1:B:30:GLU:HG2	1.95	0.67
1:A:276:GLY:N	2:A:601:XAP:H22	2.10	0.67
1:A:90:ALA:HB3	1:B:398:ASN:HD21	1.59	0.66
1:A:195:SER:HB2	1:A:233:ASP:HB3	1.76	0.66
1:A:291:ILE:CG2	1:B:116:GLN:HG3	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLY:H	2:A:601:XAP:C1	2.09	0.65
1:B:222:GLY:HA3	1:B:229:MET:HE2	1.80	0.63
1:A:33:SER:O	1:A:34:SER:C	2.37	0.62
1:A:276:GLY:H	2:A:601:XAP:C2	2.12	0.62
1:A:398:ASN:HD21	1:B:90:ALA:HB3	1.64	0.62
1:A:346:PRO:O	1:A:347:ASP:HB2	1.99	0.62
1:A:90:ALA:HB3	1:B:398:ASN:ND2	2.15	0.61
1:A:236:GLY:HA3	2:A:601:XAP:H21	1.84	0.60
1:B:348:GLU:O	1:B:349:LYS:HB3	2.01	0.60
1:A:67:ALA:HA	1:A:88:ASP:HB3	1.83	0.60
1:B:222:GLY:HA3	1:B:229:MET:HE3	1.83	0.59
1:A:138:GLU:OE1	1:A:141:LYS:NZ	2.32	0.58
1:A:296:VAL:HG23	1:A:313:THR:OG1	2.04	0.58
1:A:291:ILE:HG21	1:B:116:GLN:HG3	1.85	0.58
1:A:277:ARG:HG2	2:A:601:XAP:C1	2.34	0.58
1:B:67:ALA:HA	1:B:88:ASP:HB3	1.85	0.58
1:B:346:PRO:O	1:B:347:ASP:HB2	2.04	0.57
1:A:24:LEU:HD11	1:A:287:ALA:HB2	1.85	0.57
1:B:216:ARG:HD3	1:B:262:TYR:O	2.04	0.57
1:B:183:ARG:O	1:B:187:LEU:HG	2.06	0.56
1:A:216:ARG:HD3	1:A:262:TYR:O	2.06	0.56
1:A:388:ALA:O	1:A:390:THR:HG23	2.05	0.56
1:A:115:LYS:NZ	1:A:138:GLU:OE2	2.29	0.56
1:A:398:ASN:ND2	1:B:90:ALA:HB3	2.20	0.56
1:B:401:GLN:HA	1:B:401:GLN:OE1	2.07	0.55
1:A:110:TYR:HB3	1:A:131:MET:HG2	1.89	0.55
1:A:16:GLU:HG3	1:A:17:GLY:H	1.70	0.55
1:B:117:VAL:HG22	1:B:141:LYS:HG2	1.89	0.55
1:B:243:ASP:OD2	1:B:337:LYS:HE2	2.06	0.55
1:B:73:SER:HB2	1:B:76:ILE:HG12	1.88	0.55
1:A:77:VAL:HG12	1:A:101:LEU:HD12	1.89	0.54
1:A:93:THR:HG21	1:B:401:GLN:NE2	2.22	0.54
1:B:52:HIS:CD2	1:B:83:THR:HG21	2.43	0.54
1:A:348:GLU:O	1:A:349:LYS:HB3	2.07	0.53
1:B:148:LYS:HA	1:B:148:LYS:HE2	1.91	0.53
1:A:148:LYS:HA	1:A:148:LYS:HE2	1.90	0.52
1:B:208:PHE:CD2	1:B:255:ILE:HD11	2.44	0.52
1:A:401:GLN:OE1	1:A:401:GLN:HA	2.10	0.52
1:B:110:TYR:HB3	1:B:131:MET:HG2	1.91	0.52
1:A:330:LEU:HD23	1:B:330:LEU:HD23	1.91	0.51
1:A:208:PHE:CD2	1:A:255:ILE:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLY:HA3	1:A:229:MET:CE	2.40	0.51
1:A:173:THR:HB	1:A:175:ARG:HH11	1.76	0.50
1:A:320:ASP:O	1:A:366:ILE:HD11	2.10	0.50
1:B:296:VAL:HG23	1:B:313:THR:OG1	2.12	0.50
1:B:389:TYR:HE2	2:B:601:XAP:HN22	1.58	0.50
1:B:202:CYS:SG	1:B:202:CYS:O	2.70	0.50
1:A:367:VAL:HG11	1:A:370:CYS:HB3	1.94	0.49
1:A:90:ALA:CB	1:B:398:ASN:HD21	2.25	0.49
1:B:110:TYR:CE1	1:B:115:LYS:HG2	2.48	0.49
1:B:24:LEU:HD11	1:B:287:ALA:HB2	1.92	0.49
1:B:205:PRO:CB	1:B:254:VAL:HG21	2.42	0.49
1:B:16:GLU:HG3	1:B:17:GLY:N	2.26	0.48
1:A:24:LEU:HD21	1:A:382:LEU:CD1	2.42	0.48
1:A:222:GLY:HA3	1:A:229:MET:HE2	1.96	0.47
1:B:52:HIS:CD2	1:B:83:THR:CG2	2.98	0.47
1:B:320:ASP:OD2	1:B:325:SER:HB2	2.15	0.47
1:B:237:GLY:H	2:B:601:XAP:C2	2.25	0.47
1:A:134:ASP:CG	1:B:294:LYS:HZ1	2.19	0.47
1:A:37:LYS:HZ2	1:A:378:GLY:HA2	1.79	0.47
1:B:39:ALA:HA	1:B:287:ALA:O	2.15	0.47
1:B:110:TYR:CZ	1:B:115:LYS:HG2	2.50	0.47
1:A:322:VAL:O	1:A:327:ASN:HA	2.15	0.46
1:B:289:ASN:O	1:B:291:ILE:HG23	2.14	0.46
1:A:110:TYR:CZ	1:A:115:LYS:HG2	2.49	0.46
1:A:154:ARG:HA	1:A:195:SER:O	2.15	0.46
1:A:243:ASP:OD2	1:A:337:LYS:HE2	2.16	0.46
1:A:205:PRO:HB2	1:A:254:VAL:HG21	1.96	0.46
1:B:136:GLU:HG3	1:B:137:VAL:N	2.31	0.46
1:A:52:HIS:CG	1:A:83:THR:HG21	2.51	0.46
1:A:291:ILE:HG22	1:B:116:GLN:HG3	1.98	0.46
1:A:52:HIS:CD2	1:A:83:THR:HG21	2.52	0.45
1:A:346:PRO:O	1:A:347:ASP:CB	2.64	0.45
1:A:112:ASN:HA	1:A:113:PRO:HD3	1.83	0.45
1:A:320:ASP:OD2	1:A:325:SER:HB2	2.16	0.45
1:A:37:LYS:HZ2	1:A:378:GLY:CA	2.29	0.45
1:B:348:GLU:O	1:B:349:LYS:CB	2.64	0.45
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.74	0.45
1:B:173:THR:HB	1:B:175:ARG:HH11	1.82	0.44
1:A:135:SER:HB3	1:B:294:LYS:HG2	1.98	0.44
1:A:49:LEU:HD13	1:A:49:LEU:HA	1.88	0.44
1:A:8:GLU:HA	1:A:8:GLU:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLU:O	1:B:141:LYS:HB2	2.17	0.44
1:B:183:ARG:NH2	1:B:186:GLU:HG3	2.33	0.44
1:A:34:SER:HB3	1:A:35:ASP:H	1.66	0.44
1:A:350:TYR:CE2	1:A:373:PRO:HD3	2.53	0.44
1:B:204:ASP:OD2	1:B:206:GLU:HB2	2.17	0.44
1:B:205:PRO:HB2	1:B:254:VAL:HG21	1.99	0.44
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.84	0.43
1:A:398:ASN:HD21	1:B:90:ALA:CB	2.30	0.43
1:A:364:ASP:HB3	1:B:169:LYS:HZ2	1.83	0.43
1:B:24:LEU:HD21	1:B:382:LEU:HD13	2.00	0.43
1:A:143:ALA:HB2	1:A:189:ILE:HD11	2.00	0.43
1:A:319:ASN:N	1:A:319:ASN:OD1	2.46	0.43
1:A:90:ALA:HB1	1:A:112:ASN:HB2	2.00	0.43
1:A:197:HIS:CE1	1:A:236:GLY:H	2.36	0.43
1:A:275:PRO:HG2	1:A:279:TYR:HE2	1.83	0.43
1:B:84:GLY:HA2	1:B:107:ARG:NH2	2.34	0.43
1:A:92:LYS:HG3	1:A:122:TYR:CG	2.54	0.43
1:B:346:PRO:O	1:B:347:ASP:CB	2.66	0.43
1:A:136:GLU:HG3	1:A:137:VAL:N	2.34	0.43
1:A:24:LEU:HD21	1:A:382:LEU:HD13	2.01	0.43
1:B:412:PRO:O	1:B:415:GLN:HB2	2.19	0.43
1:A:237:GLY:H	2:A:601:XAP:H21	1.84	0.42
1:B:112:ASN:HA	1:B:113:PRO:HD3	1.89	0.42
1:A:345:LYS:HB3	1:A:346:PRO:HD2	2.00	0.42
1:B:130:MET:SD	1:B:231:LEU:HD13	2.60	0.42
1:A:52:HIS:CD2	1:A:83:THR:CG2	3.03	0.42
1:B:24:LEU:HD12	1:B:40:PHE:CE2	2.55	0.42
1:A:198:VAL:HG13	1:A:207:THR:HG21	2.01	0.42
1:A:282:SER:HA	1:A:385:ASN:HA	2.01	0.42
2:B:601:XAP:H22	2:B:601:XAP:HN21	1.65	0.42
1:B:200:SER:C	1:B:202:CYS:H	2.23	0.41
1:B:8:GLU:HA	1:B:8:GLU:OE1	2.20	0.41
1:A:276:GLY:H	2:A:601:XAP:H11	1.84	0.41
1:A:41:TYR:CD1	1:A:284:PHE:HD2	2.38	0.41
1:B:412:PRO:O	1:B:413:ALA:C	2.58	0.41
1:B:115:LYS:HE2	1:B:115:LYS:HB2	1.94	0.41
1:B:278:TYR:H	2:B:601:XAP:HN12	1.67	0.41
1:B:132:THR:HA	1:B:152:VAL:O	2.21	0.41
1:B:341:GLN:HG2	1:B:380:TRP:HB2	2.01	0.41
1:A:73:SER:HB2	1:A:76:ILE:HG12	2.02	0.41
1:B:199:GLY:O	1:B:202:CYS:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:THR:HG22	1:B:352:SER:HB3	2.03	0.41
1:A:183:ARG:NH2	1:A:186:GLU:HG3	2.36	0.41
1:A:24:LEU:HD12	1:A:40:PHE:CE2	2.55	0.41
1:A:80:LEU:HD22	1:A:85:THR:HG21	2.02	0.41
1:B:90:ALA:HB1	1:B:112:ASN:HB2	2.02	0.41
1:A:110:TYR:CE1	1:A:115:LYS:HG2	2.56	0.40
1:B:135:SER:OG	1:B:138:GLU:HB2	2.21	0.40
1:B:326:PHE:CE2	1:B:366:ILE:HD13	2.57	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	386/461 (84%)	350 (91%)	30 (8%)	6 (2%)	9 40
1	B	386/461 (84%)	350 (91%)	31 (8%)	5 (1%)	12 45
All	All	772/922 (84%)	700 (91%)	61 (8%)	11 (1%)	11 43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	34	SER
1	A	347	ASP
1	B	35	ASP
1	B	347	ASP
1	B	33	SER
1	B	34	SER
1	B	16	GLU
1	A	16	GLU
1	A	32	SER

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Mol	Chain	Res	Type
1	A	134	ASP

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	332/391 (85%)	298 (90%)	34 (10%)	7 28
1	B	332/391 (85%)	304 (92%)	28 (8%)	11 38
All	All	664/782 (85%)	602 (91%)	62 (9%)	9 33

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	28	ILE
1	A	30	GLU
1	A	33	SER
1	A	34	SER
1	A	35	ASP
1	A	36	ASP
1	A	50	LYS
1	A	53	LEU
1	A	74	LYS
1	A	78	LYS
1	A	93	THR
1	A	110	TYR
1	A	136	GLU
1	A	148	LYS
1	A	175	ARG
1	A	176	THR
1	A	195	SER
1	A	202	CYS
1	A	225	VAL
1	A	231	LEU
1	A	247	LYS

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Mol	Chain	Res	Type
1	A	254	VAL
1	A	296	VAL
1	A	311	GLU
1	A	341	GLN
1	A	352	SER
1	A	363	LEU
1	A	369	ARG
1	A	374	GLU
1	A	391	VAL
1	A	398	ASN
1	A	404	THR
1	A	418	GLN
1	B	7	GLU
1	B	16	GLU
1	B	28	ILE
1	B	30	GLU
1	B	36	ASP
1	B	50	LYS
1	B	53	LEU
1	B	74	LYS
1	B	110	TYR
1	B	136	GLU
1	B	148	LYS
1	B	175	ARG
1	B	176	THR
1	B	195	SER
1	B	202	CYS
1	B	225	VAL
1	B	247	LYS
1	B	296	VAL
1	B	311	GLU
1	B	341	GLN
1	B	345	LYS
1	B	352	SER
1	B	363	LEU
1	B	369	ARG
1	B	398	ASN
1	B	404	THR
1	B	415	GLN
1	B	418	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	96	GLN
1	A	99	GLN
1	A	125	ASN
1	A	197	HIS
1	A	333	HIS
1	A	385	ASN
1	A	398	ASN
1	A	401	GLN
1	A	418	GLN
1	B	29	ASN
1	B	96	GLN
1	B	197	HIS
1	B	333	HIS
1	B	385	ASN
1	B	398	ASN
1	B	401	GLN
1	B	418	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	XAP	A	601	-	3,5,5	0.19	0	3,4,4	0.98	0
2	XAP	B	601	-	3,5,5	0.23	0	3,4,4	1.17	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	XAP	A	601	-	-	1/2/3/3	-
2	XAP	B	601	-	-	1/2/3/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	XAP	C1-C2-C3-O1
2	B	601	XAP	N1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	XAP	12	0
2	B	601	XAP	10	0

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, 95^{th} 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	392/461 (85%)	-0.31	10 (2%) 56 27	10, 27, 60, 79	0
1	B	392/461 (85%)	-0.29	9 (2%) 60 31	10, 28, 60, 81	0
All	All	784/922 (85%)	-0.30	19 (2%) 59 30	10, 28, 60, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	GLU	4.4
1	A	311	GLU	4.0
1	A	346	PRO	3.7
1	B	311	GLU	3.6
1	A	347	ASP	3.3
1	B	34	SER	2.9
1	B	346	PRO	2.8
1	B	421	GLN	2.8
1	B	33	SER	2.7
1	A	32	SER	2.6
1	A	33	SER	2.4
1	B	10	ASP	2.3
1	B	7	GLU	2.3
1	A	203	THR	2.3
1	A	266	ASP	2.1
1	A	34	SER	2.1
1	B	201	GLY	2.1
1	A	8	GLU	2.0
1	A	15	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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(Å^2)	Q<0.9
2	XAP	A	601	6/6	0.94	0.17	16,18,19,20	0
2	XAP	B	601	6/6	0.95	0.17	28,28,29,30	0

6.5 Other polymers (i)

There are no such residues in this entry.