



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:01 PM UTC

PDB ID : 2ON3 / pdb_00002on3
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

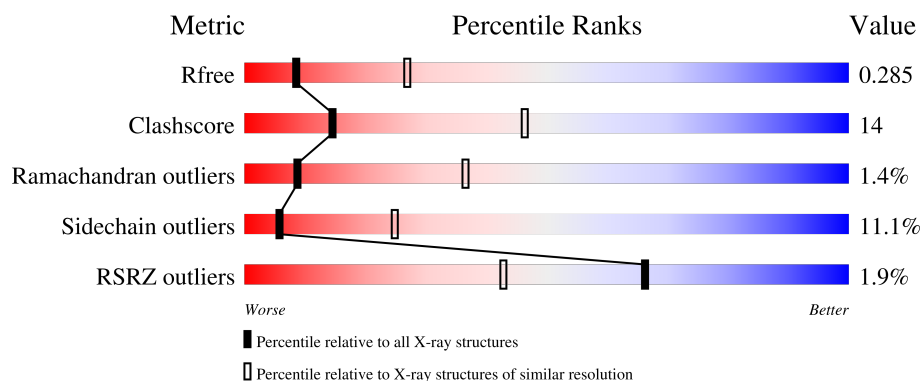
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	461	
1	B	461	

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 [i](#)

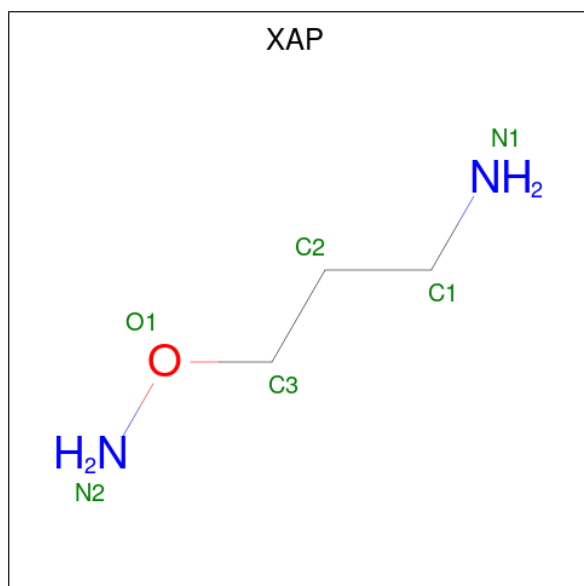
There are 2 unique types of molecules in this entry. The entry contains 6158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-AMINOXY-1-AMINOPROPANE (CCD ID: XAP) (formula: C₃H₁₀N₂O).

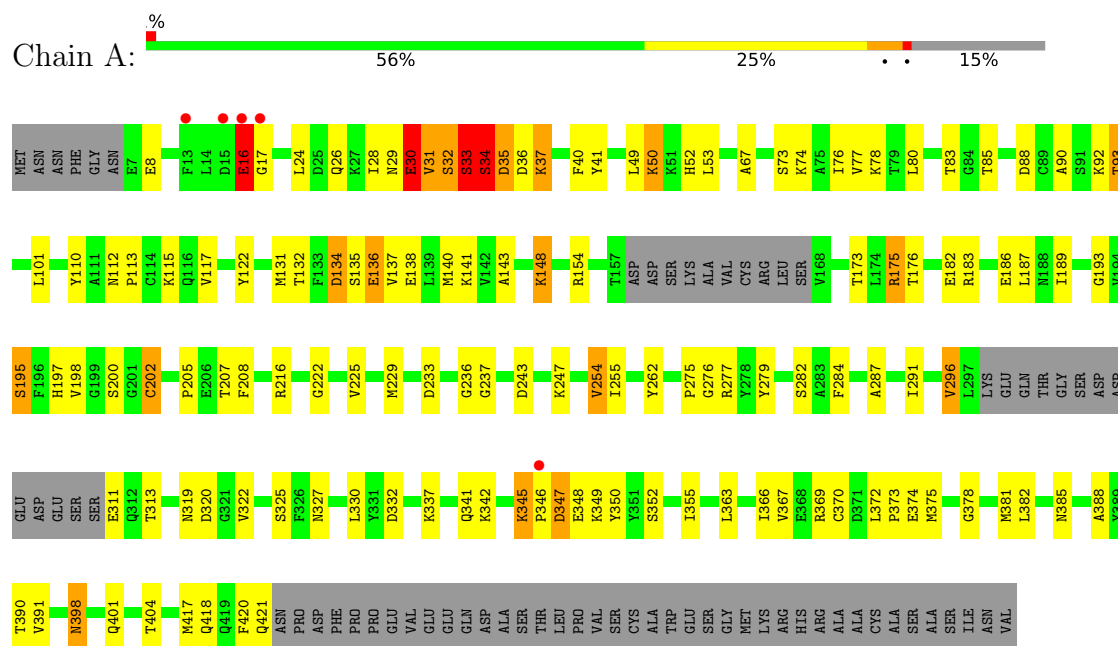


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			6	3	2	1		
2	B	1	Total	C	N	O	0	0
			6	3	2	1		

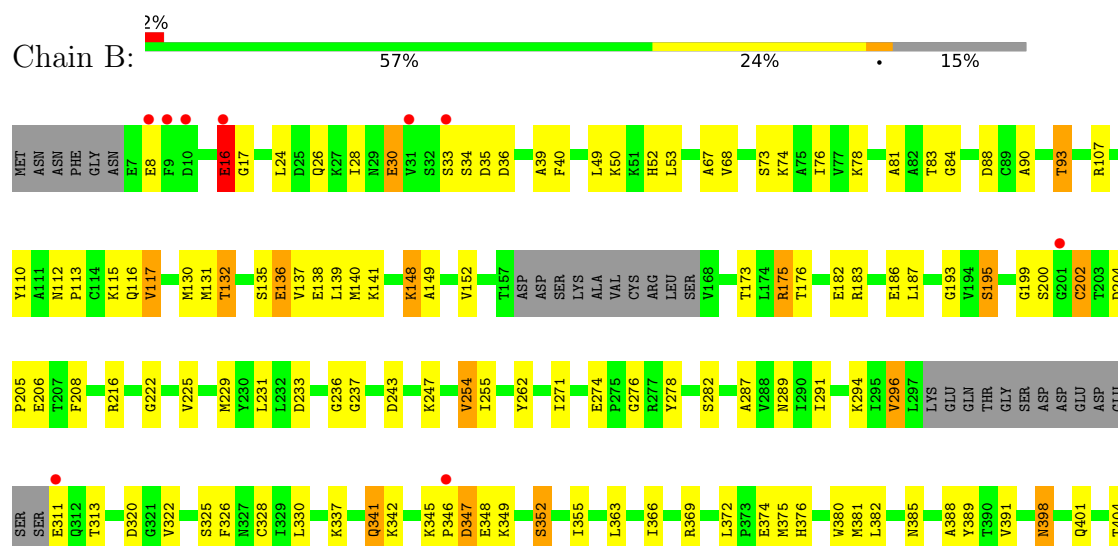
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Ornithine decarboxylase



• Molecule 1: Ornithine decarboxylase



P412	A413	V414	Q415	Q418	Q421	ASN	PRO	ASP	PHE	PRO	PRO	GLU	VAL	GLU	GLU	GLN	ASP	ALA	SER	THR	LEU	PRO	VAL	SER	CYS	ALA	ALA	TRP	GLU	SER	GLY	MET	LYS	ARG	HIS	ARG	ALA	ALA	CYS	ALA	SER	ALA	SER	ILE	ASN	VAL
------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

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) 99.6 (19.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

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	0.83	1/3142 (0.0%)	1.06	5/4253 (0.1%)
1	B	0.84	2/3142 (0.1%)	1.03	7/4253 (0.2%)
All	All	0.84	3/6284 (0.0%)	1.04	12/8506 (0.1%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	322	VAL	CA-CB	6.57	1.62	1.54
1	A	37	LYS	CA-C	-5.83	1.45	1.53
1	B	388	ALA	CA-CB	-5.23	1.45	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	GLY	N-CA-C	8.63	122.56	110.74
1	B	193	GLY	N-CA-C	8.07	121.80	110.74
1	A	31	VAL	CB-CA-C	-7.95	102.27	111.09
1	A	37	LYS	N-CA-C	-6.74	99.04	108.54
1	A	117	VAL	N-CA-C	6.66	118.21	110.62
1	A	30	GLU	N-CA-C	-6.37	105.38	113.02
1	B	274	GLU	CA-C-N	-6.33	113.43	120.14
1	B	274	GLU	C-N-CA	-6.33	113.43	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	VAL	N-CA-C	6.05	117.51	110.62
1	B	81	ALA	N-CA-C	-5.45	105.03	110.97
1	B	376	HIS	N-CA-C	5.12	117.94	109.85
1	B	149	ALA	N-CA-C	5.08	116.85	110.24

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3073	0	3043	98	0
1	B	3073	0	3043	88	0
2	A	6	0	10	12	0
2	B	6	0	10	10	0
All	All	6158	0	6106	172	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 14.

All (172) 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:B:222:GLY:HA3	1:B:229:MET:HE3	1.47	0.95
1:A:401:GLN:HE21	1:B:93:THR:HG21	1.32	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:H	2:A:601:XAP:H11	1.33	0.92
1:A:222:GLY:HA3	1:A:229:MET:HE3	1.51	0.91
1:A:277:ARG:N	2:A:601:XAP:H11	1.88	0.87
1:A:140:MET:HE2	1:A:183:ARG:HH11	1.43	0.82
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: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:222:GLY:HA3	1:B:229:MET:CE	2.15	0.74
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:HG12	1:A:31:VAL:O	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:A:33:SER:O	1:A:34:SER:C	2.37	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
1:A:276:GLY:H	2:A:601:XAP:C1	2.09	0.65
1:A:115:LYS:NZ	1:A:138:GLU:OE2	2.29	0.63
1:A:276:GLY:H	2:A:601:XAP:C2	2.12	0.62
1:B:355:ILE:HG12	1:B:381:MET:HE1	1.80	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:B:140:MET:HE2	1:B:183:ARG:HH11	1.65	0.60
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:140:MET:HE2	1:A:183:ARG:NH1	2.16	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:398:ASN:ND2	1:B:90:ALA:HB3	2.20	0.56
1:B:372:LEU:HD13	1:B:375:MET:HE2	1.88	0.55
1:A:16:GLU:HG3	1:A:17:GLY:H	1.70	0.55
1:A:110:TYR:HB3	1:A:131:MET:HG2	1.89	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:401:GLN:HA	1:B:401:GLN:OE1	2.07	0.53
1:B:148:LYS:HE2	1:B:148:LYS:HA	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:HA	1:A:401:GLN:OE1	2.10	0.52
1:B:110:TYR:HB3	1:B:131:MET:HG2	1.91	0.52
1:A:355:ILE:HG12	1:A:381:MET:HE1	1.92	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
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:O	1:B:202:CYS:SG	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:A:134:ASP:CG	1:B:294:LYS:HZ1	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD21	1:A:382:LEU:CD1	2.42	0.48
1:A:372:LEU:HD13	1:A:375:MET:HE2	1.96	0.48
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: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:B:412:PRO:O	1:B:413:ALA:C	2.58	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:B:200:SER:C	1:B:202:CYS:H	2.23	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:B:348:GLU:O	1:B:349:LYS:CB	2.64	0.45
1:A:80:LEU:HD23	1:A:80:LEU:HA	1.74	0.45
1:B:88:ASP:OD1	1:B:88:ASP:C	2.60	0.44
1:A:135:SER:HB3	1:B:294:LYS:HG2	1.98	0.44
1:B:173:THR:HB	1:B:175:ARG:HH11	1.82	0.44
1:A:8:GLU:HA	1:A:8:GLU:OE1	2.17	0.44
1:A:49:LEU:HD13	1:A:49:LEU:HA	1.88	0.44
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:200:SER:C	1:A:202:CYS:H	2.26	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:HD23	1:A:187:LEU:HA	1.84	0.43
1:A:398:ASN:HD21	1:B:90:ALA:CB	2.30	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:OD1	1:A:319:ASN:N	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ALA:HB1	1:A:112:ASN:HB2	2.00	0.43
1:B:67:ALA:O	1:B:68:VAL:C	2.62	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:49:LEU:O	1:A:50:LYS:C	2.61	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:24:LEU:HD21	1:A:382:LEU:HD13	2.01	0.43
1:A:136:GLU:HG3	1:A:137:VAL:N	2.34	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:B:140:MET:HE2	1:B:183:ARG:NH1	2.34	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:277:ARG:HH12	1:A:332:ASP:CG	2.27	0.42
1:A:282:SER:HA	1:A:385:ASN:HA	2.01	0.42
2:B:601:XAP:HN21	2:B:601:XAP:H22	1.65	0.42
1:B:8:GLU:HA	1:B:8:GLU:OE1	2.20	0.41
1:A:41:TYR:CD1	1:A:284:PHE:HD2	2.38	0.41
1:A:276:GLY:H	2:A:601:XAP:H11	1.84	0.41
1:A:420:PHE:O	1:A:421:GLN:C	2.63	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:326:PHE:C	1:B:328:CYS:N	2.78	0.41
1:A:32:SER:C	1:A:33:SER:O	2.64	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
1:B:313:THR:HG22	1:B:352:SER:HB3	2.03	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:A:183:ARG:NH2	1:A:186:GLU:HG3	2.36	0.41
1:B:90:ALA:HB1	1:B:112:ASN:HB2	2.02	0.41
1:B:115:LYS:NZ	1:B:138:GLU:OE2	2.51	0.41
1:A:110:TYR:CE1	1:A:115:LYS:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:C	1:A:31:VAL:H	2.30	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%)	7	34
1	B	386/461 (84%)	350 (91%)	31 (8%)	5 (1%)	9	38
All	All	772/922 (84%)	700 (91%)	61 (8%)	11 (1%)	9	36

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
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%)	295 (89%)	37 (11%)	6	25
1	B	332/391 (85%)	295 (89%)	37 (11%)	6	25
All	All	664/782 (85%)	590 (89%)	74 (11%)	6	25

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	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	132	THR
1	A	136	GLU
1	A	148	LYS
1	A	175	ARG
1	A	176	THR
1	A	182	GLU
1	A	195	SER
1	A	202	CYS
1	A	225	VAL
1	A	247	LYS
1	A	254	VAL
1	A	296	VAL
1	A	311	GLU
1	A	341	GLN
1	A	342	LYS

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Mol	Chain	Res	Type
1	A	345	LYS
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	417	MET
1	A	418	GLN
1	B	16	GLU
1	B	28	ILE
1	B	30	GLU
1	B	36	ASP
1	B	49	LEU
1	B	50	LYS
1	B	53	LEU
1	B	74	LYS
1	B	78	LYS
1	B	93	THR
1	B	132	THR
1	B	136	GLU
1	B	139	LEU
1	B	148	LYS
1	B	175	ARG
1	B	176	THR
1	B	182	GLU
1	B	195	SER
1	B	202	CYS
1	B	225	VAL
1	B	247	LYS
1	B	254	VAL
1	B	271	ILE
1	B	296	VAL
1	B	311	GLU
1	B	341	GLN
1	B	342	LYS
1	B	345	LYS
1	B	352	SER
1	B	363	LEU
1	B	369	ARG
1	B	374	GLU

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Mol	Chain	Res	Type
1	B	391	VAL
1	B	398	ASN
1	B	404	THR
1	B	415	GLN
1	B	418	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	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	96	GLN
1	B	125	ASN
1	B	129	GLN
1	B	385	ASN
1	B	398	ASN
1	B	401	GLN
1	B	418	GLN
1	B	419	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 oligosaccharides 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	0.18	0	3,4,4	1.00	0
2	XAP	B	601	-	3,5,5	0.22	0	3,4,4	1.20	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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	392/461 (85%)	-0.24	5 (1%) 75 53	10, 27, 60, 79	0
1	B	392/461 (85%)	-0.20	10 (2%) 57 34	10, 28, 60, 81	0
All	All	784/922 (85%)	-0.22	15 (1%) 66 43	10, 28, 60, 81	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	16	GLU	3.6
1	B	418	GLN	3.2
1	B	346	PRO	2.8
1	A	13	PHE	2.5
1	A	17	GLY	2.4
1	A	15	ASP	2.4
1	B	8	GLU	2.2
1	B	31	VAL	2.2
1	A	346	PRO	2.2
1	B	33	SER	2.1
1	B	10	ASP	2.1
1	B	9	PHE	2.1
1	B	201	GLY	2.1
1	A	16	GLU	2.1
1	B	311	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XAP	A	601	6/6	0.91	0.10	16,18,19,20	0
2	XAP	B	601	6/6	0.95	0.11	28,28,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.