



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:53 AM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

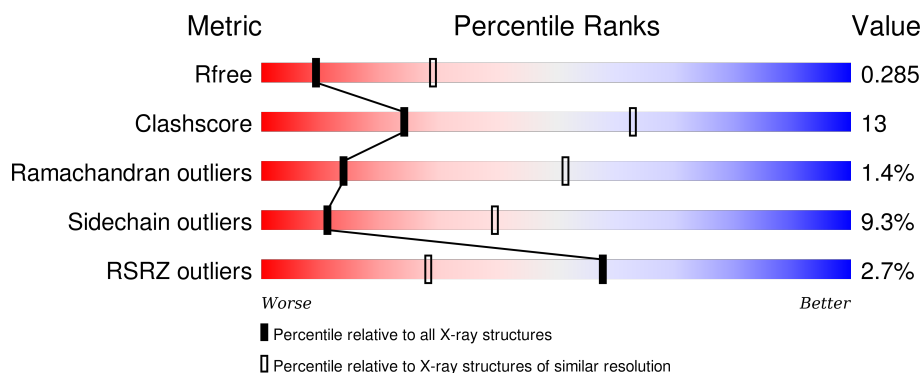
1 Overall quality at a glance ⓘ

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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	<div> <div>2%</div> <div>59%</div> <div>23%</div> <div>•</div> <div>15%</div> </div>
1	B	461	<div> <div>2%</div> <div>62%</div> <div>20%</div> <div>•</div> <div>15%</div> </div>

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](#)

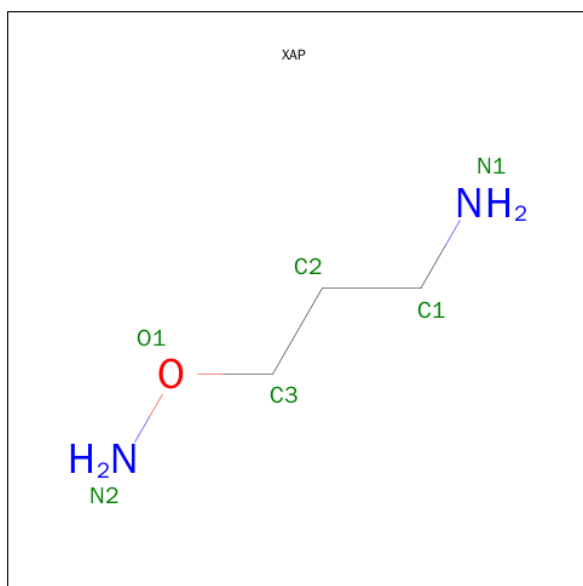
There are 2 unique types of molecules in this entry. The entry contains 6158 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (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		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- Sequence logo for Chain A. The y-axis represents information content in bits (0.00 to 0.20). The x-axis shows positions 1 to 100. A horizontal bar at the top indicates the overall conservation: 59% (green), 23% (yellow), and 15% (grey). A red dot at position 2 indicates a high conservation score.
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1 | ASP | 0.00 |
| 2 | ASP | 0.20 |
| 3 | ASP | 0.00 |
| 4 | ASP | 0.00 |
| 5 | ASP | 0.00 |
| 6 | ASP | 0.00 |
| 7 | ASP | 0.00 |
| 8 | ASP | 0.00 |
| 9 | ASP | 0.00 |
| 10 | ASP | 0.00 |
| 11 | ASP | 0.00 |
| 12 | ASP | 0.00 |
| 13 | ASP | 0.00 |
| 14 | ASP | 0.00 |
| 15 | ASP | 0.00 |
| 16 | ASP | 0.00 |
| 17 | ASP | 0.00 |
| 18 | ASP | 0.00 |
| 19 | ASP | 0.00 |
| 20 | ASP | 0.00 |
| 21 | ASP | 0.00 |
| 22 | ASP | 0.00 |
| 23 | ASP | 0.00 |
| 24 | ASP | 0.00 |
| 25 | ASP | 0.00 |
| 26 | ASP | 0.00 |
| 27 | ASP | 0.00 |
| 28 | ASP | 0.00 |
| 29 | ASP | 0.00 |
| 30 | ASP | 0.00 |
| 31 | ASP | 0.00 |
| 32 | ASP | 0.00 |
| 33 | ASP | 0.00 |
| 34 | ASP | 0.00 |
| 35 | ASP | 0.00 |
| 36 | ASP | 0.00 |
| 37 | ASP | 0.00 |
| 38 | ASP | 0.00 |
| 39 | ASP | 0.00 |
| 40 | ASP | 0.00 |
| 41 | ASP | 0.00 |
| 42 | ASP | 0.00 |
| 43 | ASP | 0.00 |
| 44 | ASP | 0.00 |
| 45 | ASP | 0.00 |
| 46 | ASP | 0.00 |
| 47 | ASP | 0.00 |
| 48 | ASP | 0.00 |
| 49 | ASP | 0.00 |
| 50 | ASP | 0.00 |
| 51 | ASP | 0.00 |
| 52 | ASP | 0.00 |
| 53 | ASP | 0.00 |
| 54 | ASP | 0.00 |
| 55 | ASP | 0.00 |
| 56 | ASP | 0.00 |
| 57 | ASP | 0.00 |
| 58 | ASP | 0.00 |
| 59 | ASP | 0.00 |
| 60 | ASP | 0.00 |
| 61 | ASP | 0.00 |
| 62 | ASP | 0.00 |
| 63 | ASP | 0.00 |
| 64 | ASP | 0.00 |
| 65 | ASP | 0.00 |
| 66 | ASP | 0.00 |
| 67 | ASP | 0.00 |
| 68 | ASP | 0.00 |
| 69 | ASP | 0.00 |
| 70 | ASP | 0.00 |
| 71 | ASP | 0.00 |
| 72 | ASP | 0.00 |
| 73 | ASP | 0.00 |
| 74 | ASP | 0.00 |
| 75 | ASP | 0.00 |
| 76 | ASP | 0.00 |
| 77 | ASP | 0.00 |
| 78 | ASP | 0.00 |
| 79 | ASP | 0.00 |
| 80 | ASP | 0.00 |
| 81 | ASP | 0.00 |
| 82 | ASP | 0.00 |
| 83 | ASP | 0.00 |
| 84 | ASP | 0.00 |
| 85 | ASP | 0.00 |
| 86 | ASP | 0.00 |
| 87 | ASP | 0.00 |
| 88 | ASP | 0.00 |
| 89 | ASP | 0.00 |
| 90 | ASP | 0.00 |
| 91 | ASP | 0.00 |
| 92 | ASP | 0.00 |
| 93 | ASP | 0.00 |
| 94 | ASP | 0.00 |
| 95 | ASP | 0.00 |
| 96 | ASP | 0.00 |
| 97 | ASP | 0.00 |
| 98 | ASP | 0.00 |
| 99 | ASP | 0.00 |
| 100 | ASP | 0.00 |

- Chain B:
-
- 2% 62% 20% 15%
- MET ASN ASN PHE GLY ASN E7 E8 F9 D10 E16 G17 L24 D25 Q26 R27 I28 N29 E30 S33 S34 D35 D36 A39 F40 R50 R51 R52 L53 L55 A67 S73 R74 A75 I76 T83 G84 D88 G89 A90 T93 R107 Y110 A111 N112 P113 G114 K115 Q116 V117 M229 Q341 Q342 R343 P344 P345 P346 R347 E348 K349 S352 L363 I366 R369 W380 M381 L382 N385 Y389 N398 Q401 T404 P412 A413 A414 Q415 Q418 Q421 A421 P421 P422 P423 P424 P425 P426 P427 P428 P429 P430 P431 P432 P433 P434 P435 P436 P437 P438 P439 P440 P441 P442 P443 P444 P445 P446 P447 P448 P449 P450 P451 P452 P453 P454 P455 P456 P457 P458 P459 P460 P461 P462 P463 P464 P465 P466 P467 P468 P469 P470 P471 P472 P473 P474 P475 P476 P477 P478 P479 P480 P481 P482 P483 P484 P485 P486 P487 P488 P489 P490 P491 P492 P493 P494 P495 P496 P497 P498 P499 P500 P501 P502 P503 P504 P505 P506 P507 P508 P509 P510 P511 P512 P513 P514 P515 P516 P517 P518 P519 P520 P521 P522 P523 P524 P525 P526 P527 P528 P529 P530 P531 P532 P533 P534 P535 P536 P537 P538 P539 P540 P541 P542 P543 P544 P545 P546 P547 P548 P549 P550 P551 P552 P553 P554 P555 P556 P557 P558 P559 P560 P561 P562 P563 P564 P565 P566 P567 P568 P569 P570 P571 P572 P573 P574 P575 P576 P577 P578 P579 P580 P581 P582 P583 P584 P585 P586 P587 P588 P589 P590 P591 P592 P593 P594 P595 P596 P597 P598 P599 P600 P601 P602 P603 P604 P605 P606 P607 P608 P609 P610 P611 P612 P613 P614 P615 P616 P617 P618 P619 P620 P621 P622 P623 P624 P625 P626 P627 P628 P629 P630 P631 P632 P633 P634 P635 P636 P637 P638 P639 P640 P641 P642 P643 P644 P645 P646 P647 P648 P649 P650 P651 P652 P653 P654 P655 P656 P657 P658 P659 P660 P661 P662 P663 P664 P665 P666 P667 P668 P669 P670 P671 P672 P673 P674 P675 P676 P677 P678 P679 P680 P681 P682 P683 P684 P685 P686 P687 P688 P689 P690 P691 P692 P693 P694 P695 P696 P697 P698 P699 P700 P701 P702 P703 P704 P705 P706 P707 P708 P709 P710 P711 P712 P713 P714 P715 P716 P717 P718 P719 P720 P721 P722 P723 P724 P725 P726 P727 P728 P729 P730 P731 P732 P733 P734 P735 P736 P737 P738 P739 P740 P741 P742 P743 P744 P745 P746 P747 P748 P749 P750 P751 P752 P753 P754 P755 P756 P757 P758 P759 P760 P761 P762 P763 P764 P765 P766 P767 P768 P769 P770 P771 P772 P773 P774 P775 P776 P777 P778 P779 P780 P781 P782 P783 P784 P785 P786 P787 P788 P789 P790 P791 P792 P793 P794 P795 P796 P797 P798 P799 P800 P801 P802 P803 P804 P805 P806 P807 P808 P809 P810 P811 P812 P813 P814 P815 P816 P817 P818 P819 P820 P821 P822 P823 P824 P825 P826 P827 P828 P829 P830 P831 P832 P833 P834 P835 P836 P837 P838 P839 P840 P841 P842 P843 P844 P845 P846 P847 P848 P849 P850 P851 P852 P853 P854 P855 P856 P857 P858 P859 P860 P861 P862 P863 P864 P865 P866 P867 P868 P869 P870 P871 P872 P873 P874 P875 P876 P877 P878 P879 P880 P881 P882 P883 P884 P885 P886 P887 P888 P889 P890 P891 P892 P893 P894 P895 P896 P897 P898 P899 P900 P901 P902 P903 P904 P905 P906 P907 P908 P909 P910 P911 P912 P913 P914 P915 P916 P917 P918 P919 P920 P921 P922 P923 P924 P925 P926 P927 P928 P929 P930 P931 P932 P933 P934 P935 P936 P937 P938 P939 P940 P941 P942 P943 P944 P945 P946 P947 P948 P949 P950 P951 P952 P953 P954 P955 P956 P957 P958 P959 P960 P961 P962 P963 P964 P965 P966 P967 P968 P969 P970 P971 P972 P973 P974 P975 P976 P977 P978 P979 P980 P981 P982 P983 P984 P985 P986 P987 P988 P989 P990 P991 P992 P993 P994 P995 P996 P997 P998 P999

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) 100.0 (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 (11.11%)	DCC
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 , 30.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 18056 reflections	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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 [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	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:B:237:GLY:N	2:B:601:XAP:H12	2.03	0.73
1:A:93:THR:HG21	1:B:401:GLN:HE21	1.52	0.73
1:B:276:GLY:N	2:B:601:XAP:HN11	1.85	0.73
1:A:37:LYS:NZ	1:A:378:GLY:O	2.21	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

Continued on next page...

Continued from previous page...

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:398:ASN:ND2	1:B:90:ALA:HB3	2.20	0.56
1:A:115:LYS:NZ	1:A:138:GLU:OE2	2.29	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:93:THR:HG21	1:B:401:GLN:NE2	2.22	0.54
1:A:77:VAL:HG12	1:A:101:LEU:HD12	1.89	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:222:GLY:HA3	1:A:229:MET:CE	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:389:TYR:HE2	2:B:601:XAP:HN22	1.58	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: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: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:A:134:ASP:CG	1:B:294:LYS:HZ1	2.19	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: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:B:183:ARG:NH2	1:B:186:GLU:HG3	2.33	0.44
1:B:138:GLU:O	1:B:141:LYS:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:364:ASP:HB3	1:B:169:LYS:HZ2	1.83	0.43
1:A:187:LEU:HA	1:A:187:LEU:HD23	1.84	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:B:346:PRO:O	1:B:347:ASP:CB	2.66	0.43
1:A:92:LYS:HG3	1:A:122:TYR:CG	2.54	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:24:LEU:HD12	1:B:40:PHE:CE2	2.55	0.42
1:A:52:HIS:CD2	1:A:83:THR:CG2	3.03	0.42
1:A:282:SER:HA	1:A:385:ASN:HA	2.01	0.42
1:A:198:VAL:HG13	1:A:207:THR:HG21	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:HB2	1:B:115:LYS:HE2	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:B:313:THR:HG22	1:B:352:SER:HB3	2.03	0.41
1:B:199:GLY:O	1:B:202:CYS:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:SER:HB2	1:A:76:ILE:HG12	2.02	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: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%)	12	48
1	B	386/461 (84%)	350 (91%)	31 (8%)	5 (1%)	15	53
All	All	772/922 (84%)	700 (91%)	61 (8%)	11 (1%)	14	51

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

Continued on next page...

Continued from previous page...

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%)	9	33
1	B	332/391 (85%)	304 (92%)	28 (8%)	14	45
All	All	664/782 (85%)	602 (91%)	62 (9%)	11	39

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

Continued on next page...

Continued from previous page...

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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.23	0	2,4,4	0.76	0
2	XAP	B	601	-	3,5,5	0.26	0	2,4,4	1.14	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	-	-	0/2/3/3	0/0/0/0
2	XAP	B	601	-	-	0/2/3/3	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 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%)	-0.31	11 (2%) 56 27	10, 27, 60, 79	0
1	B	392/461 (85%)	-0.28	10 (2%) 59 29	10, 28, 60, 81	0
All	All	784/922 (85%)	-0.29	21 (2%) 58 28	10, 28, 60, 81	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	GLU	4.7
1	A	311	GLU	4.0
1	B	311	GLU	3.8
1	A	346	PRO	3.7
1	A	347	ASP	3.3
1	B	34	SER	3.0
1	B	346	PRO	2.9
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	7	GLU	2.4
1	B	10	ASP	2.4
1	A	203	THR	2.3
1	A	266	ASP	2.3
1	B	201	GLY	2.1
1	A	34	SER	2.1
1	B	343	ARG	2.1
1	A	15	ASP	2.1
1	A	8	GLU	2.1
1	A	297	LEU	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	XAP	B	601	6/6	0.96	0.17	0.17	28,28,29,30	0
2	XAP	A	601	6/6	0.94	0.17	-0.05	16,18,19,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.